

=> b reg

FILE 'REGISTRY' ENTERED AT 17:08:17 ON 21 APR 2004  
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STRUCTURE FILE UPDATES: 19 APR 2004 HIGHEST RN 676225-08-4  
DICTIONARY FILE UPDATES: 19 APR 2004 HIGHEST RN 676225-08-4

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

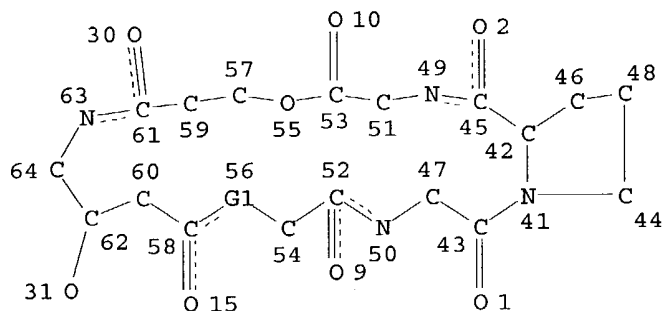
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more  
information enter HELP PROP at an arrow prompt in the file or refer  
to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> d que 157

L57

STR



VAR G1=N/O

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 31

STEREO ATTRIBUTES: NONE

=> b hcaplus

FILE 'HCAPLUS' ENTERED AT 17:08:30 ON 21 APR 2004  
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FILE COVERS 1907 - 21 Apr 2004 VOL 140 ISS 17  
FILE LAST UPDATED: 20 Apr 2004 (20040420/ED)

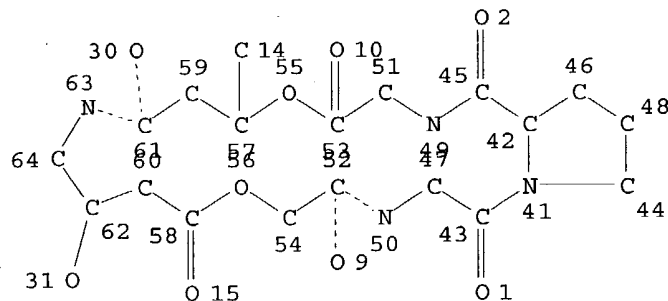
This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> d que 162

L53

STR



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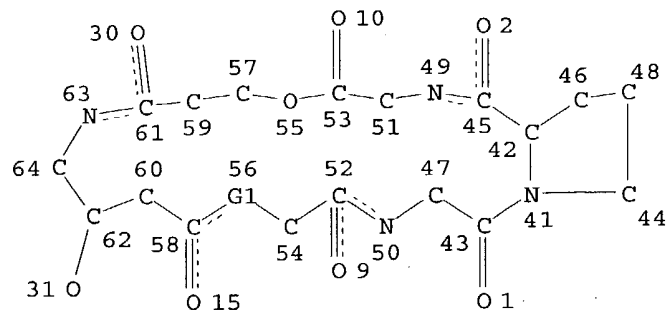
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STEREO ATTRIBUTES: NONE

L55 57 SEA FILE=REGISTRY SSS FUL L53

L56 10 SEA FILE=HCAPLUS ABB=ON PLU=ON L55

L57 STR



VAR G1=N/O

NODE ATTRIBUTES:

Searched by P. Ruppel

DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED

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RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 31

STEREO ATTRIBUTES: NONE

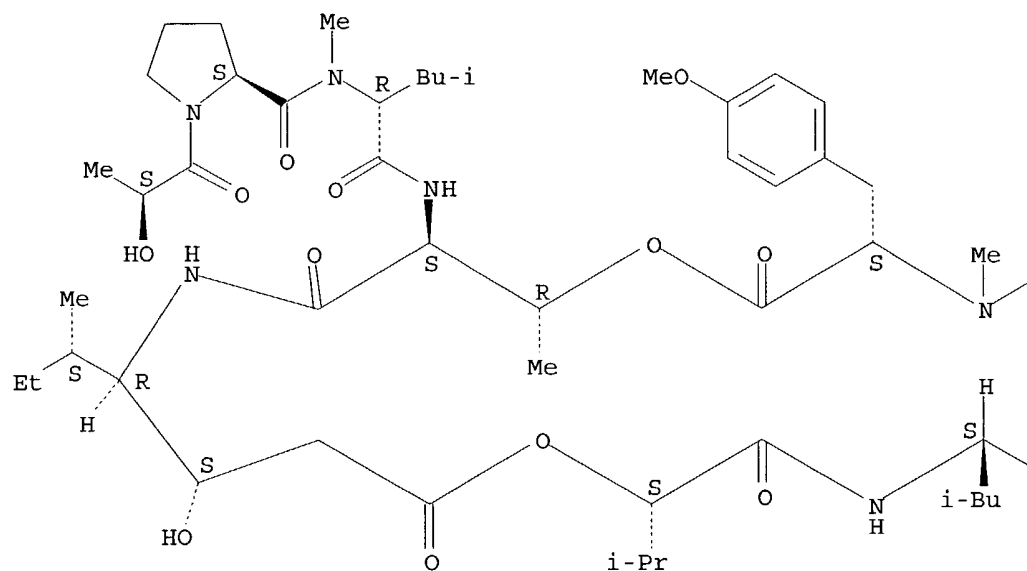
L59 68 SEA FILE=REGISTRY SSS FUL L57  
L60 11 SEA FILE=REGISTRY ABB=ON PLU=ON L59 NOT L55  
L61 2 SEA FILE=HCAPLUS ABB=ON PLU=ON L60  
L62 10 SEA FILE=HCAPLUS ABB=ON PLU=ON L56 OR L61

=> d ibib abs hitstr l62 1-10

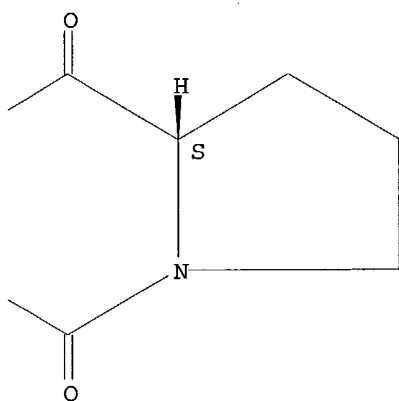
L62 ANSWER 1 OF 10 HCAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 2002:898771 HCAPLUS  
DOCUMENT NUMBER: 138:86871  
TITLE: Chemical defense in ascidians of the Didemnidae Family  
AUTHOR(S): Jollie, Madeleine M.; Leonard, Michael S.; Portonovo,  
Padma; Liang, Bo; Ding, Xiaobin; La Clair, James J.  
CORPORATE SOURCE: Department of Chemistry, University of Pennsylvania,  
Philadelphia, PA, 19104-6323, USA  
SOURCE: Bioconjugate Chemistry (2003), 14(1), 30-37  
CODEN: BCCHES; ISSN: 1043-1802  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Fluorescent analogs (DB1 and TA1) of the secondary metabolites didemnin B  
(DB) and tamandarin A (TA) were synthesized to investigate the potential  
chemical defense mechanisms of tunicates in the family Didemnidae. These  
compds. were found to alter predator-prey relations. Five species of  
freshwater fish and one marine fish, the damselfish Amphiprion ocellaris,  
were acclimated to a diet of mosquito larvae. Fish showed an immediate,  
neg. reaction to mosquito larvae treated with  $\geq 5$  ng of DB1 or TA1,  
with consumption of larvae resulting in regurgitation. Both freshwater  
and marine fish learned to avoid tainted prey by associating species of larvae  
with "distaste". Distaste for a given organism also arose when  
depsipeptides DB1 or TA1 were transferred to the fish from the surrounding  
medium. Fluorescence microscopy in fish indicated that a similar  
processing and localization followed ingestion and absorption of DB1 or  
TA1. Fluorescent labeling of DB or TA provided an ideal tool to conduct  
short-term studies of predator-prey relationships between fish and marine  
invertebrate larvae.  
IT 250211-78-0, Tamandarin A  
RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(chemical defense mechanisms of tunicates)  
RN 250211-78-0 HCAPLUS  
CN Tamandarin A (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

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IT 485389-87-5

RL: BUU (Biological use, unclassified); BIOL (Biological study); USES  
(Uses)

(tamandarin A fluorescent analog; chemical defense mechanisms of  
tunicates)

RN 485389-87-5 HCAPLUS

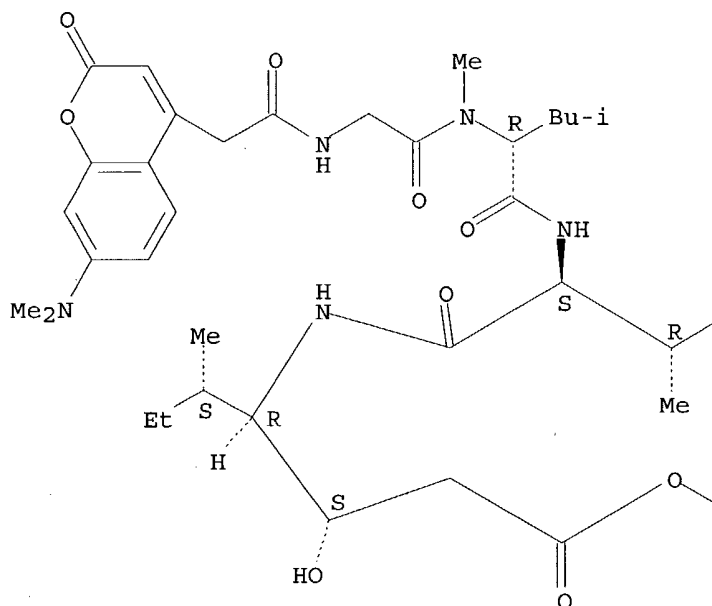
CN L-Tyrosine, N-[[7-(dimethylamino)-2-oxo-2H-1-benzopyran-4-yl]acetyl]glycyl-  
N-methyl-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-

Searched by P. Ruppel

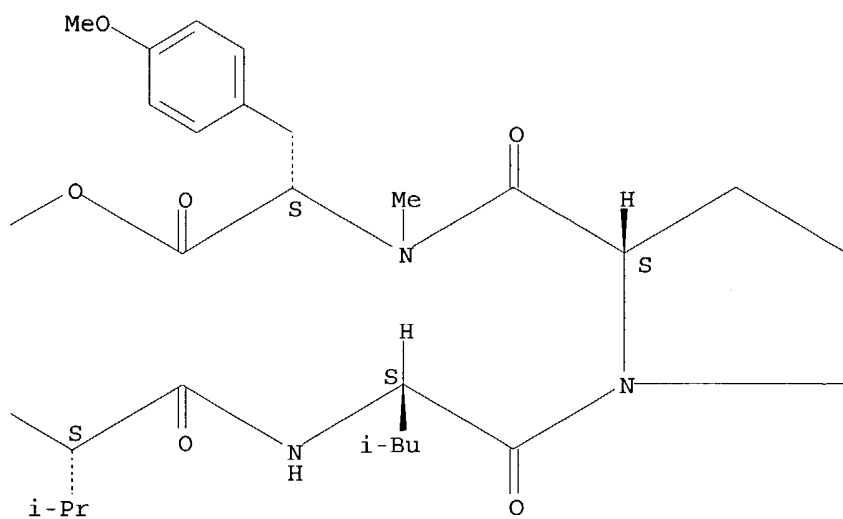
methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (8→3)-lactone (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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REFERENCE COUNT:

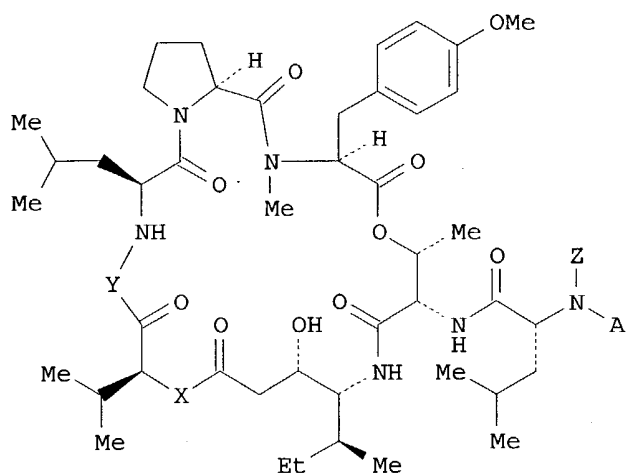
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THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Searched by P. Ruppel

L62 ANSWER 2 OF 10 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 2002:31485 HCAPLUS  
 DOCUMENT NUMBER: 136:86058  
 TITLE: Preparation of aplidine analogs as new antitumor agents  
 INVENTOR(S): Rodriguez, Ignacio; Polanco, Concepcion; Cuevas, Felix; Mandez, Paloma; Cuevas, Carmen; Gallego, Pilar; Munt, Simon; Manzanares, Ignacio  
 PATENT ASSIGNEE(S): Pharma Mar, S.A., Spain  
 SOURCE: PCT Int. Appl., 241 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002002596	A2	20020110	WO 2001-GB2901	20010702
WO 2002002596	A3	20020523		
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RW:		GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG		
EP 1294747	A2	20030326	EP 2001-945484	20010702
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BR 2001012375	A	20030624	BR 2001-12375	20010702
JP 2004502702	T2	20040129	JP 2002-507848	20010702
NO 2002006242	A	20030227	NO 2002-6242	20021227
PRIORITY APPLN. INFO.:			GB 2000-16148	A 20000630
			GB 2001-3750	A 20010215
			WO 2001-GB2901	W 20010702
OTHER SOURCE(S):		CASREACT 136:86058; MARPAT 136:86058		
GI				



I

AB Aplidine and its analogs I [ $X = CH_2, O, S, \text{ or } NR_1$ , where  $R_1 = H$ , (un)substituted alkyl, alkenyl, aryl, aralkyl;  $Y = (COR_2)_nCO$ , where  $n = 0$  or 1,  $R_2 = (un)substituted alkyl, alkenyl, aryl, aralkyl$ ;  $Z = H$ , or  $R_3CONH$ ,  $R_3CO$ , where  $R_3 = (un)substituted alkyl, alkenyl, aryl, aralkyl$ ;  $A = amino acyl, R_3SO_2$ , or  $R_3CO$ , where  $R_3 = (un)substituted alkyl, aryl, aralkyl$ ] were prepared as antitumor agents. Thus, [Val]<sub>3</sub>[Isobutyryl]<sub>8</sub>-didemnin A was prepared by multistep procedure starting from reaction of H-Leu-Pro-OCH<sub>2</sub>Ph with Boc-Val-OH (Boc = tert-butoxycarbonyl) and via coupling of Ist-Val-Leu-Pro-OBn (Ist = isostatine) intermediate with O-(Cbz-N,O-dimethyl-Tyr)-N-tert-Boc-Thr phenacyl ester (Cbz = benzyloxycarbonyl), followed by macrocyclization and coupling with Cbz-Me-D-Leu and Pyr-Pro-OH. The prepared compound was active against human lung carcinoma and human colon carcinoma.

IT 250211-78-0P, Tamandarin A 367507-55-9P

387823-42-9P 387823-43-0P 387823-44-1P

387823-45-2P 387823-56-5P 387823-59-8P

387823-61-2P 387823-62-3P 387823-82-7P

387823-84-9P 387823-85-0P 387823-86-1P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

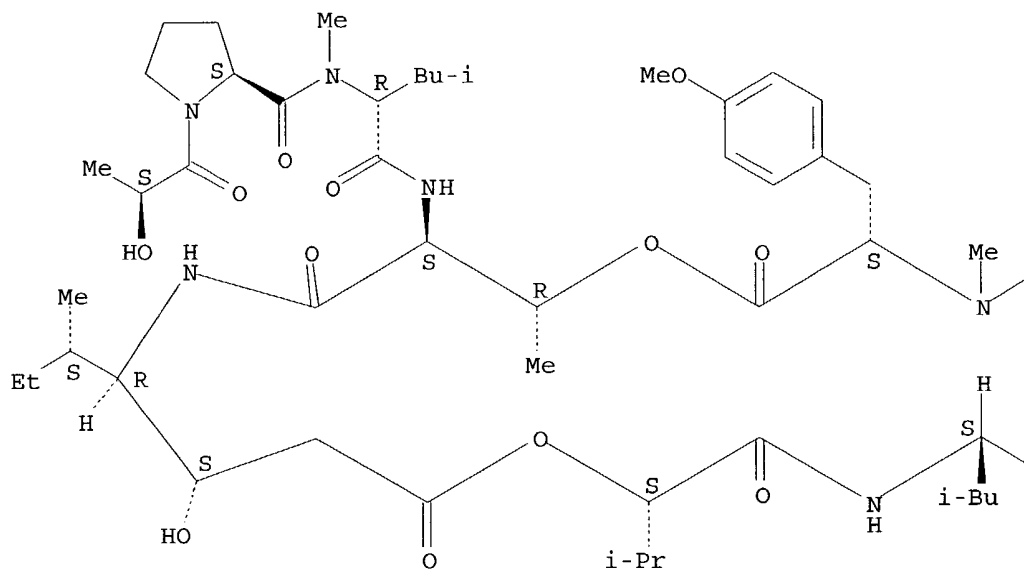
(preparation of aplidine analogs as antitumor agents)

RN 250211-78-0 HCAPLUS

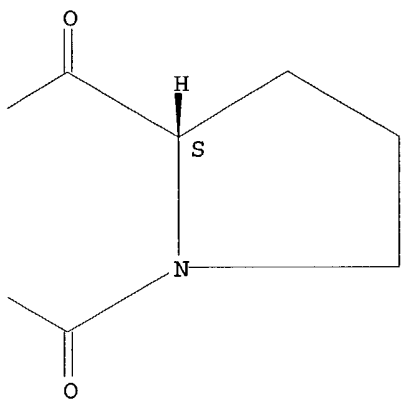
CN Tamandarin A (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

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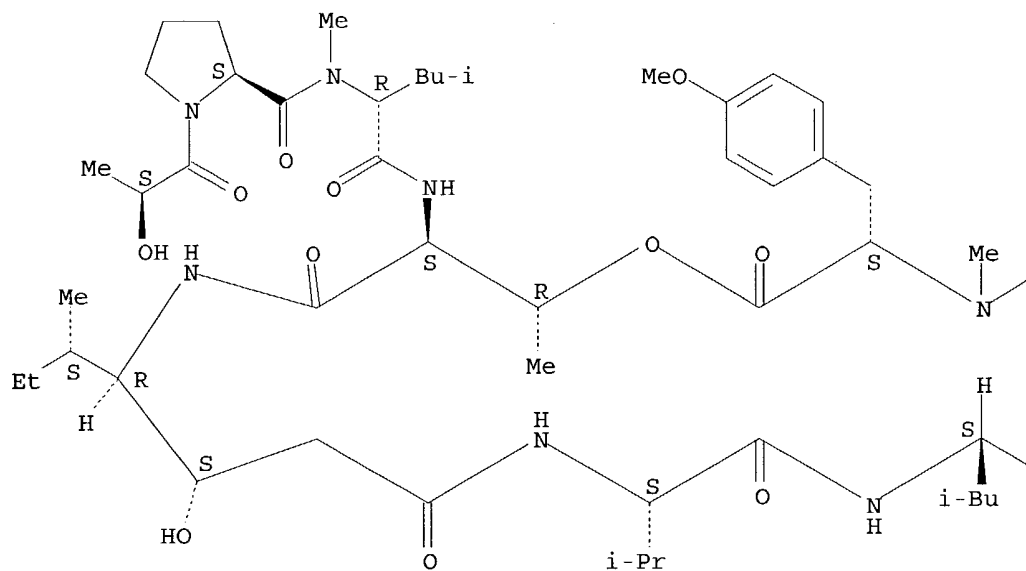
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Absolute stereochemistry.

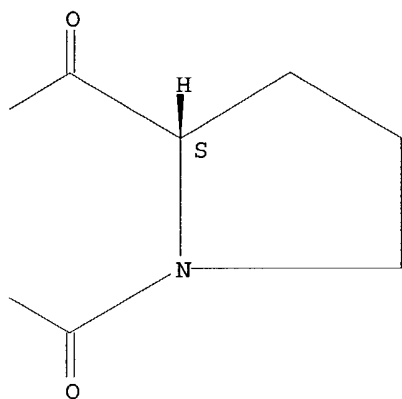
Searched by P. Ruppel



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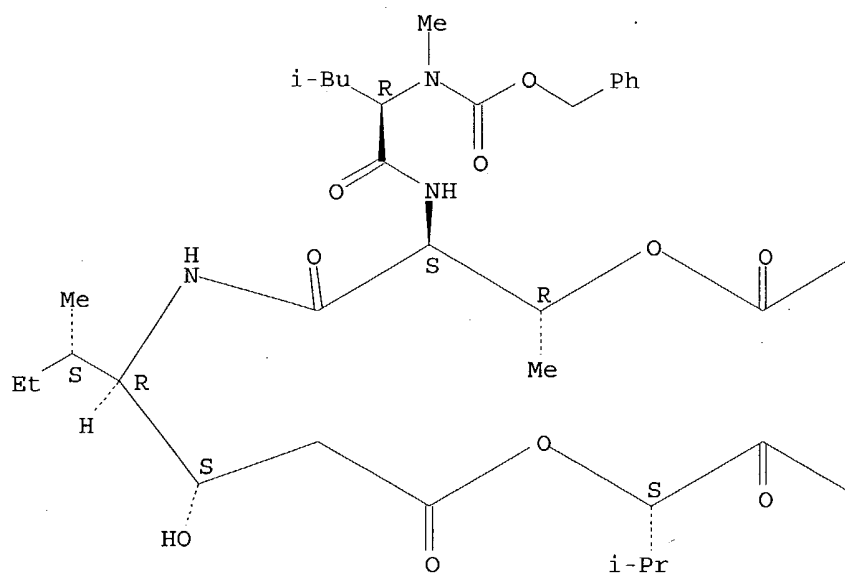


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 CN L-Tyrosine, N-methyl-N-[(phenylmethoxy) carbonyl]-D-leucyl-L-threonyl-  
 (3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-  
 methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (7→2)-lactone (9CI)  
 (CA INDEX NAME)

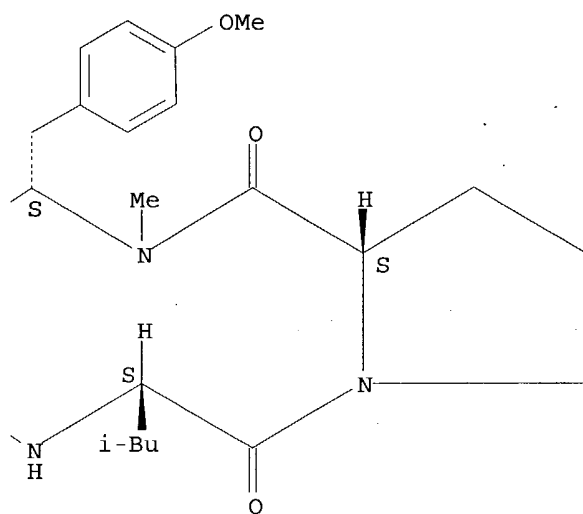
Absolute stereochemistry.

Searched by P. Ruppel

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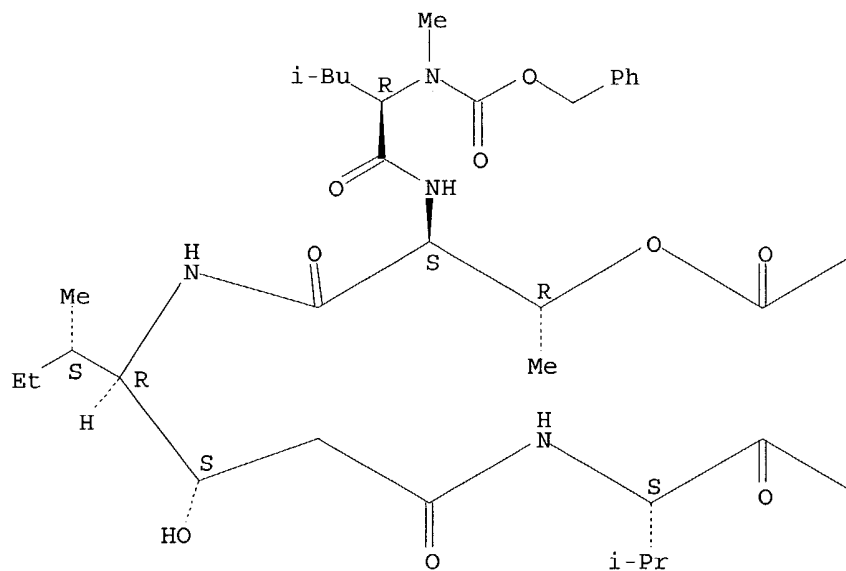
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CN L-Tyrosine, N-methyl-N-[(phenylmethoxy)carbonyl]-D-leucyl-L-threonyl-  
 (3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-L-valyl-L-leucyl-L-prolyl-  
 N,O-dimethyl-, (7 $\rightarrow$ 2)-lactone (9CI) (CA INDEX NAME)

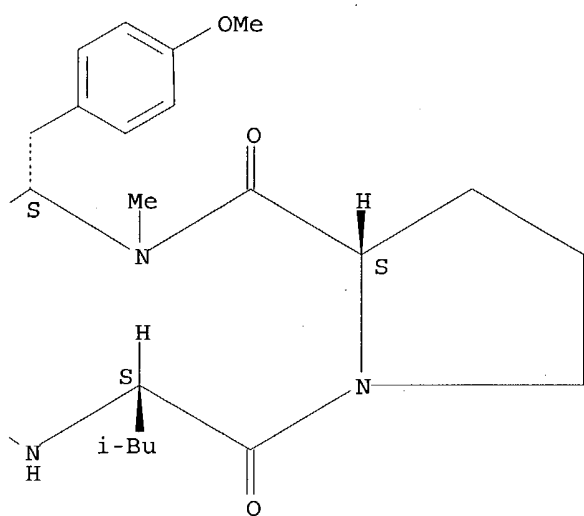
Absolute stereochemistry.

Searched by P. Ruppel

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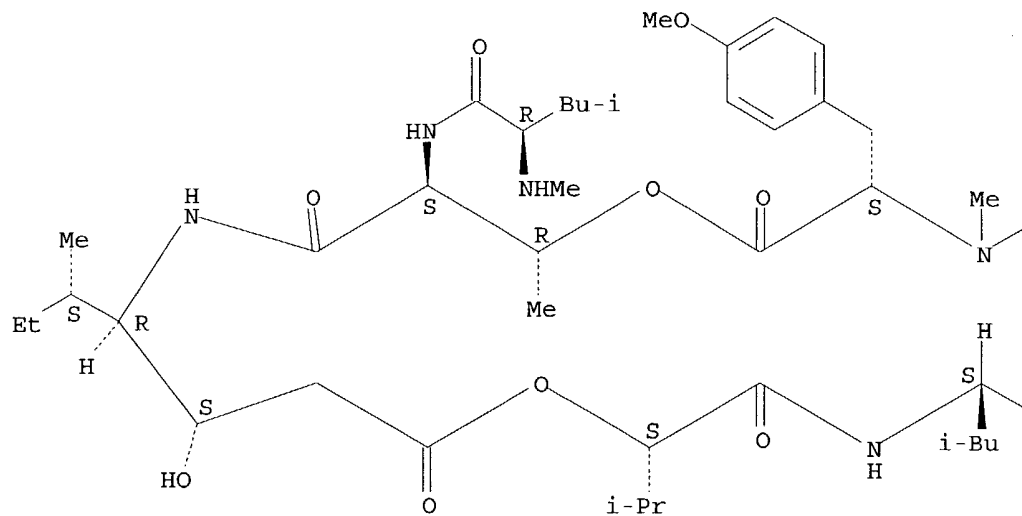
RN 387823-44-1 HCAPLUS

CN L-Tyrosine, N-methyl-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (7→2)-lactone (9CI) (CA INDEX NAME)

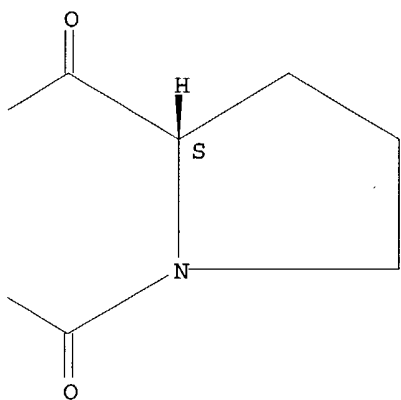
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



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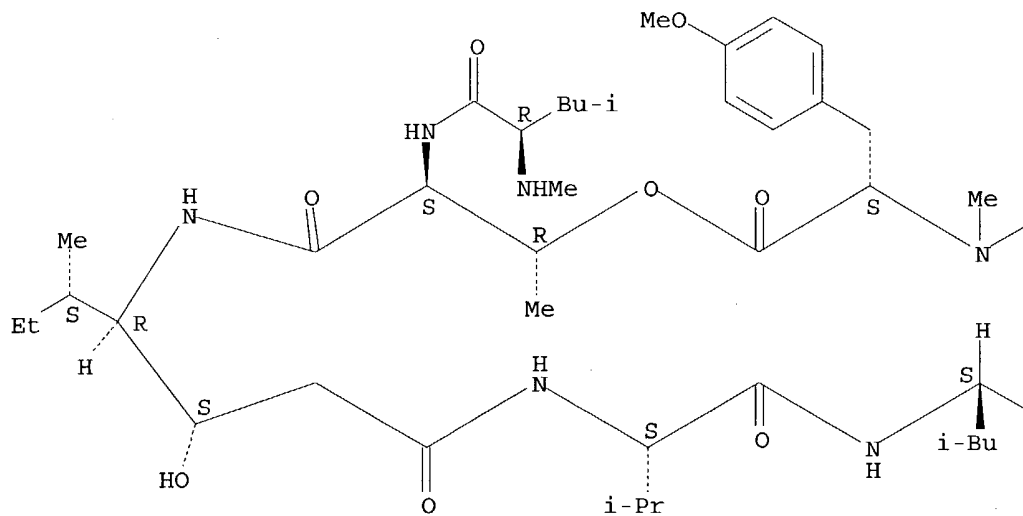


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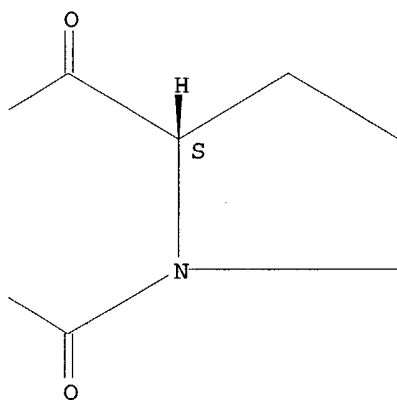
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B



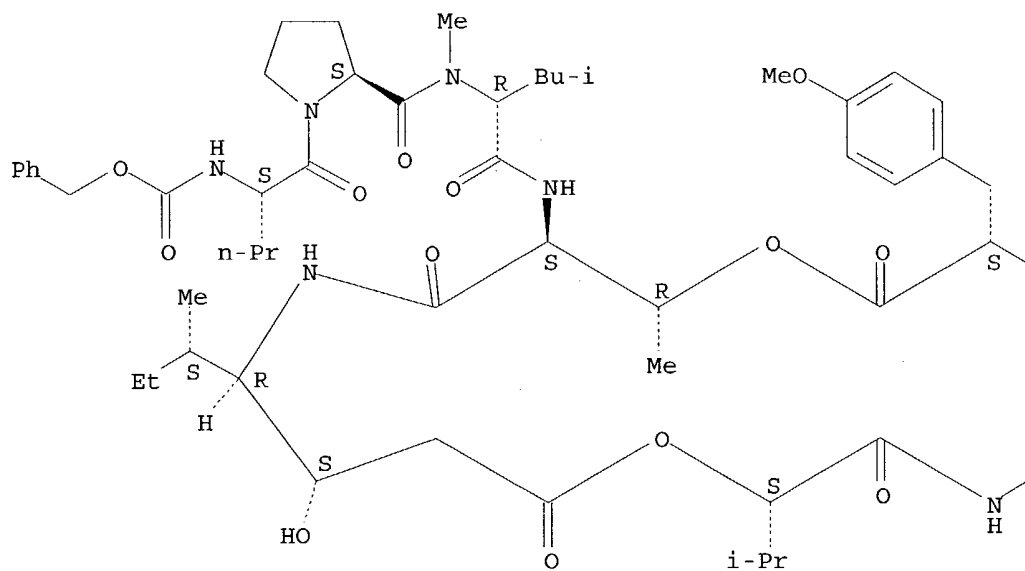
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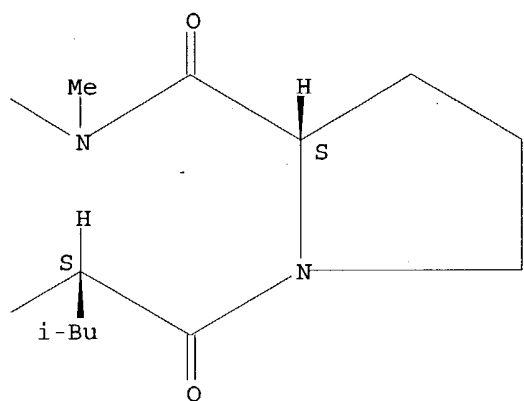
Absolute stereochemistry.

Searched by P. Ruppel

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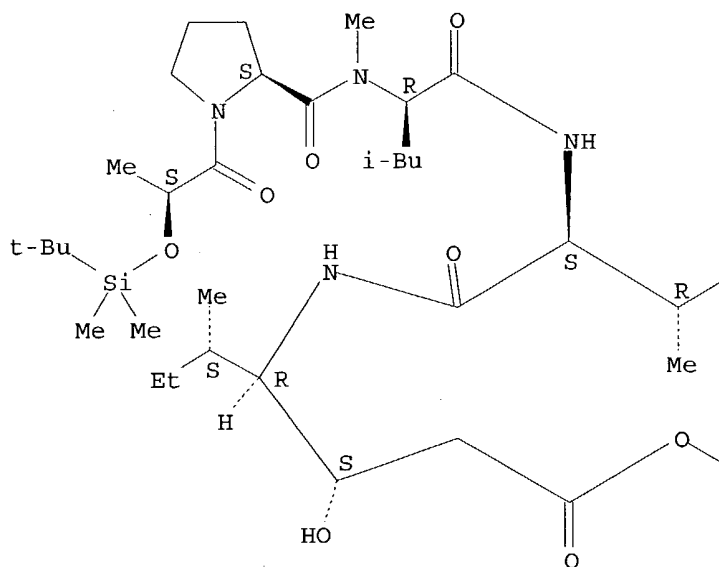
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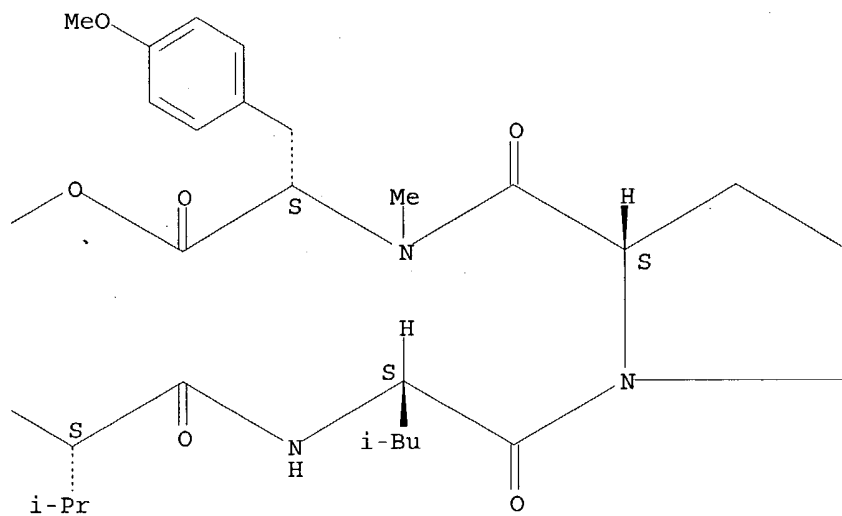
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B



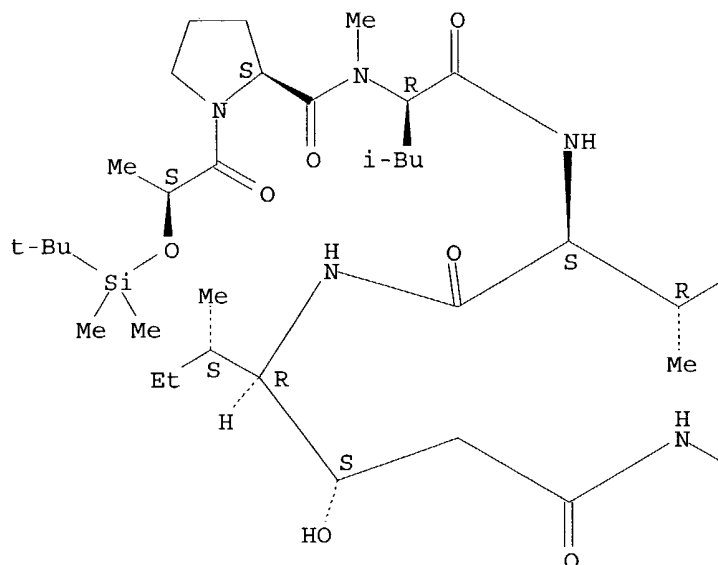
RN 387823-61-2 HCAPLUS

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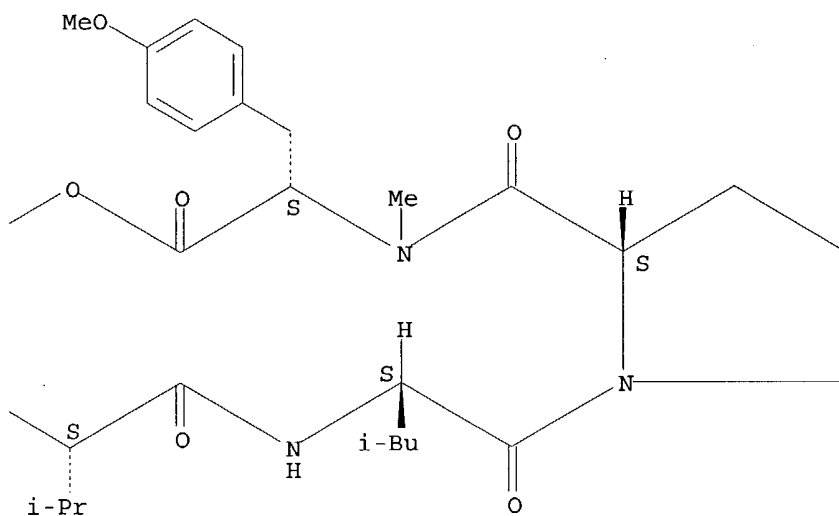
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



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RN 387823-62-3 HCAPLUS

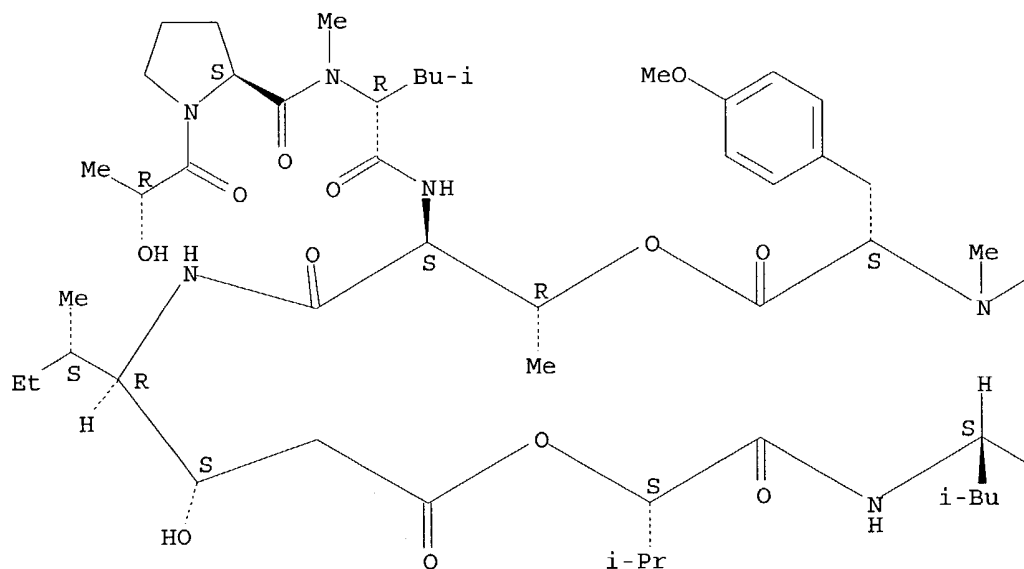
L-Tyrosine, (2R)-2-hydroxypropanoyl-L-prolyl-N-methyl-D-leucyl-L-threonyl-  
 (3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-  
 methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (9→4)-lactone (9CI)  
 (CA INDEX NAME)

Absolute stereochemistry.

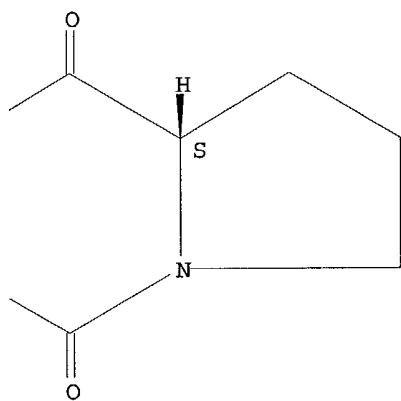
Searched by P. Ruppel



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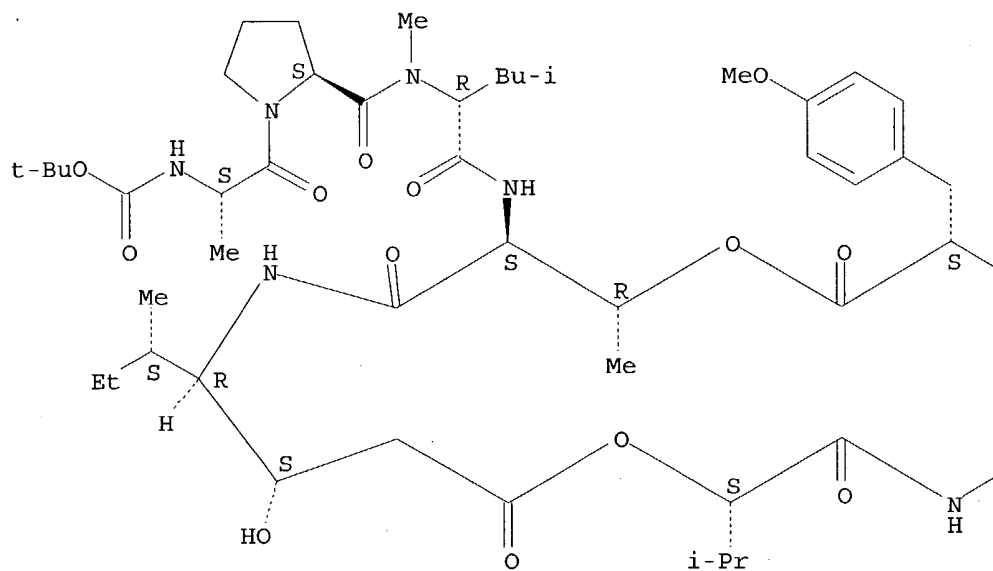
RN 387823-82-7 HCAPLUS

CN L-Tyrosine, N-[(1,1-dimethylethoxy)carbonyl]-L-alanyl-L-prolyl-N-methyl-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (9→4)-lactone (9CI) (CA INDEX NAME)

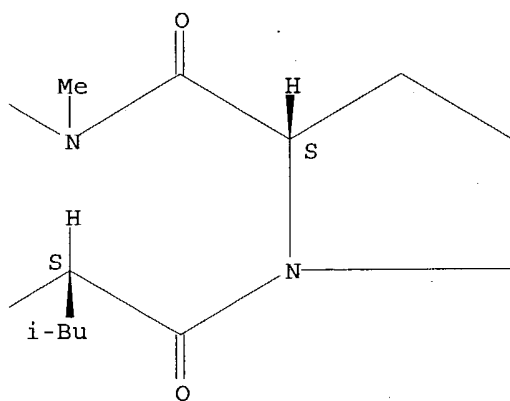
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



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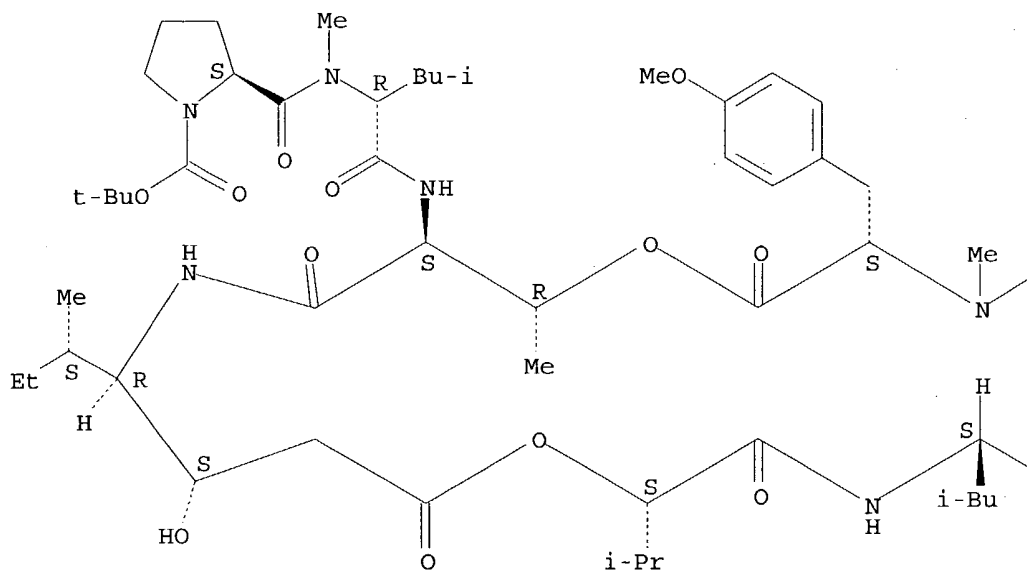


RN 387823-84-9 HCAPLUS  
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 (CA INDEX NAME)

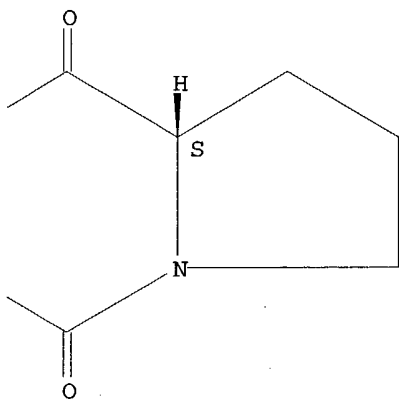
Absolute stereochemistry.

Searched by P. Ruppel

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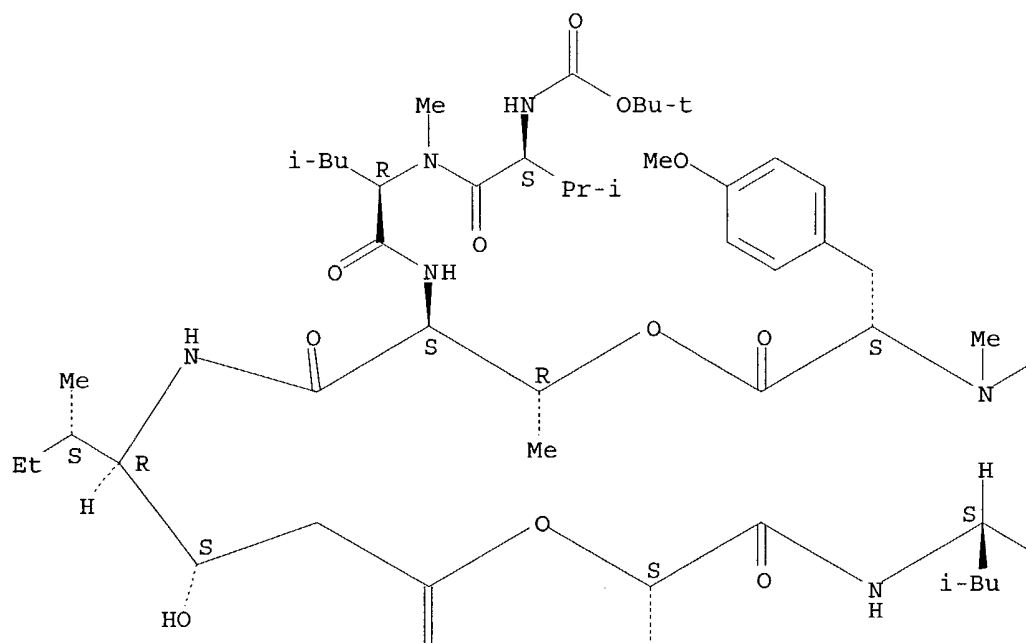
RN 387823-85-0 HCAPLUS

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(CA INDEX NAME)

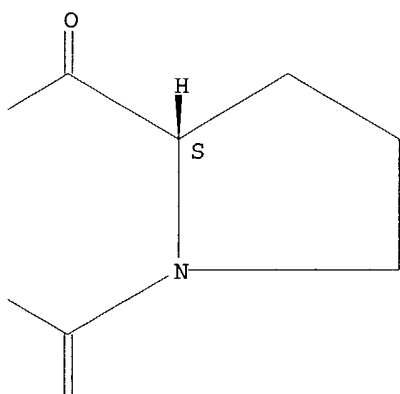
Absolute stereochemistry.

Searched by P. Ruppel

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PAGE 2-A



PAGE 2-B

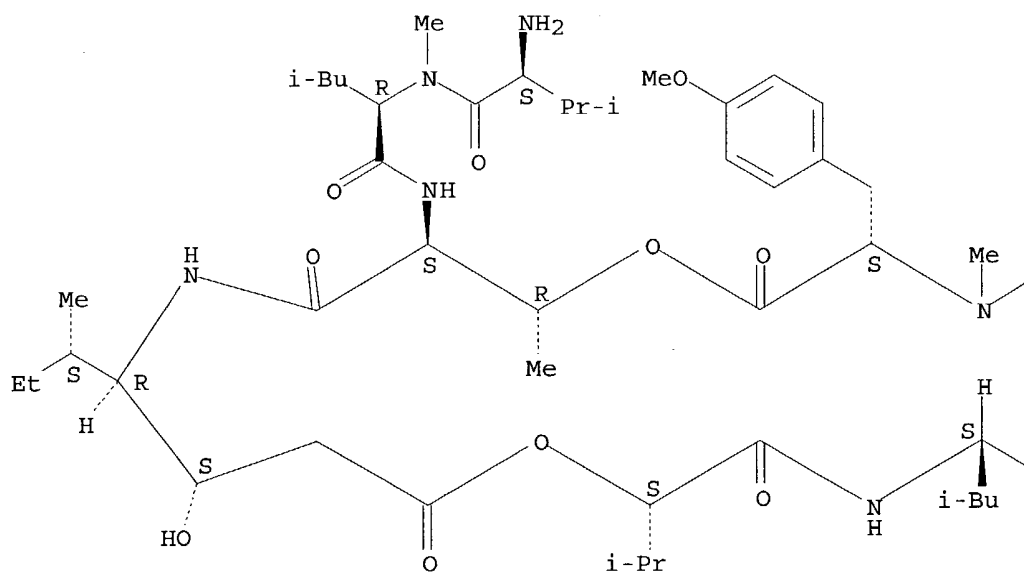


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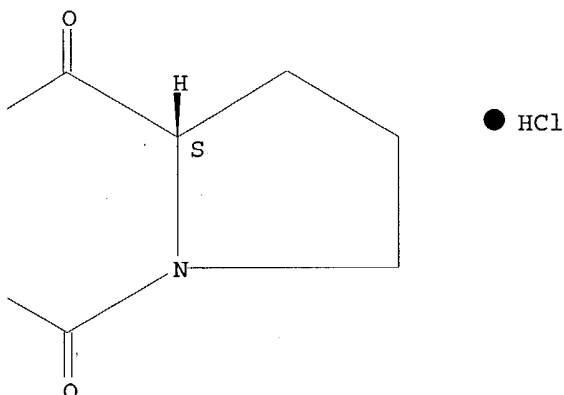
CN L-Tyrosine, L-valyl-N-methyl-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (8→3)-lactone, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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IT 345969-81-5P 367507-67-3P 387823-47-4P  
 387823-48-5P 387823-49-6P 387823-50-9P  
 387823-52-1P 387823-53-2P 387823-58-7P  
 387823-60-1P 387823-75-8P 387823-77-0P  
 387823-79-2P 387823-80-5P 387823-81-6P  
 387823-83-8P 387823-87-2P 387859-52-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
 (Uses)

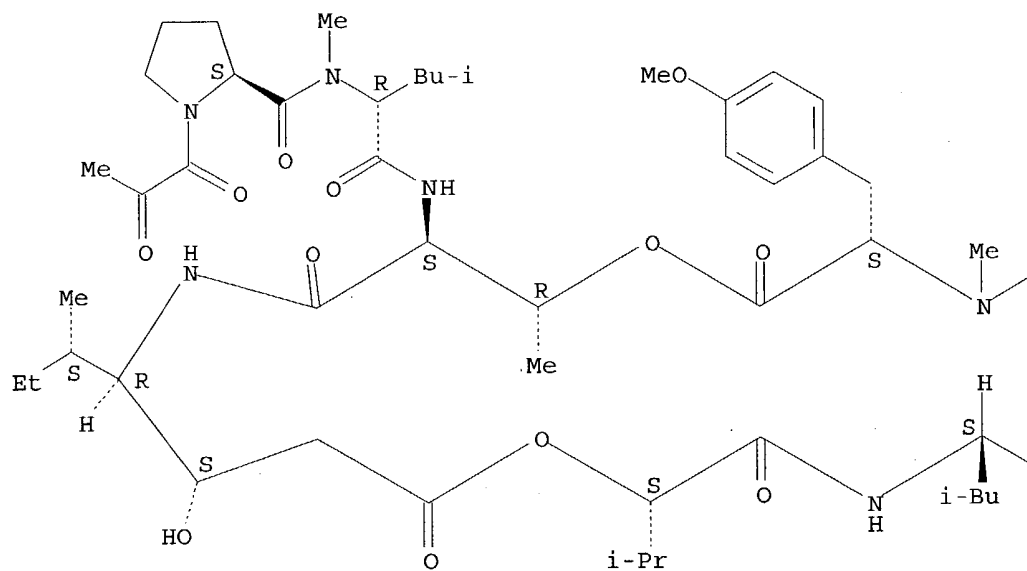
(preparation of aplidine analogs as antitumor agents)

RN 345969-81-5 HCAPLUS

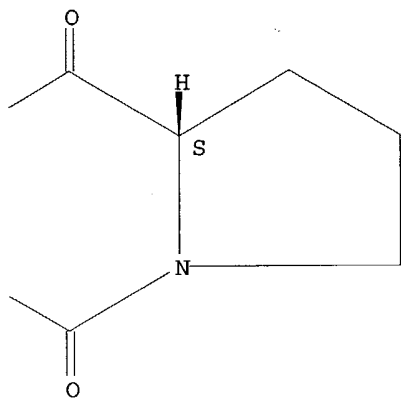
CN L-Tyrosine, 1-(1,2-dioxopropyl)-L-prolyl-N-methyl-D-leucyl-L-threonyl-  
 (3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-  
 methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (8→3)-lactone (9CI)  
 (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

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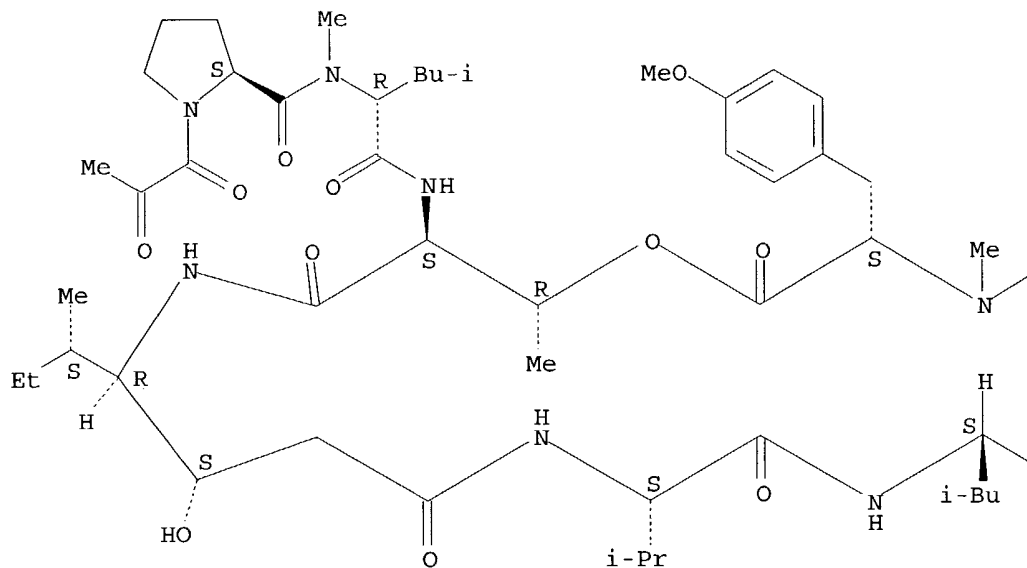


RN 367507-67-3 HCAPLUS  
 CN 2-9-Tamandarin A, 2-[1-(1,2-dioxopropyl)-L-proline]-6-L-valine- (9CI) (CA  
 INDEX NAME)

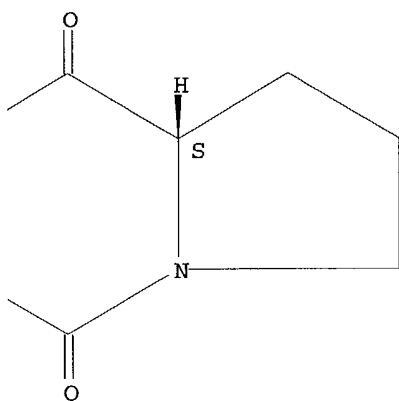
Absolute stereochemistry.

Searched by P. Ruppel

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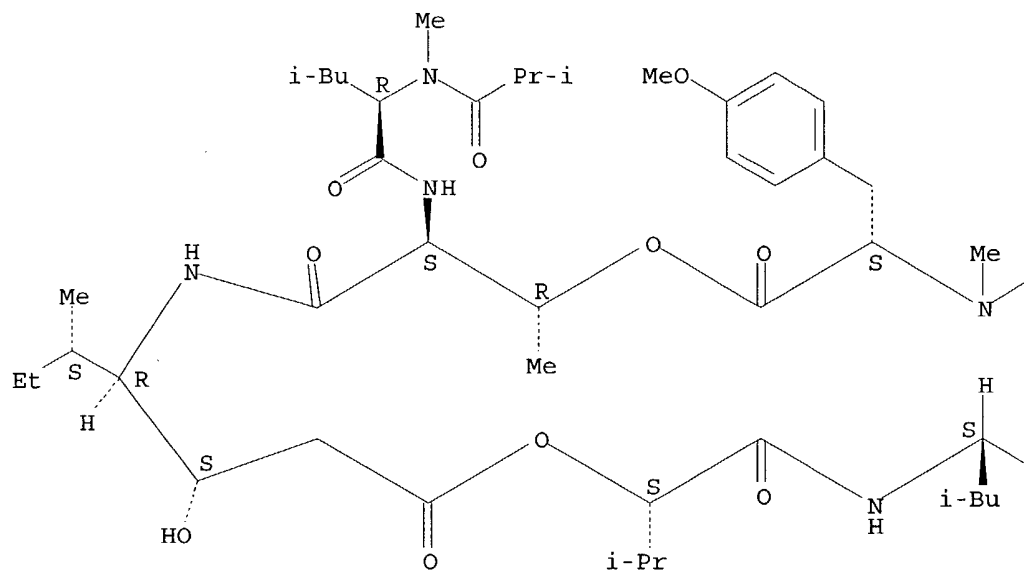
RN 387823-47-4 HCAPLUS  
 CN L-Tyrosine, N-methyl-N-(2-methyl-1-oxopropyl)-D-leucyl-L-threonyl-  
 (3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-  
 methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (7→2)-lactone (9CI)  
 (CA INDEX NAME)

Absolute stereochemistry.

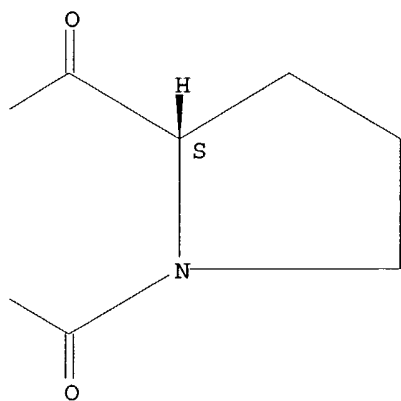
Searched by P. Ruppel



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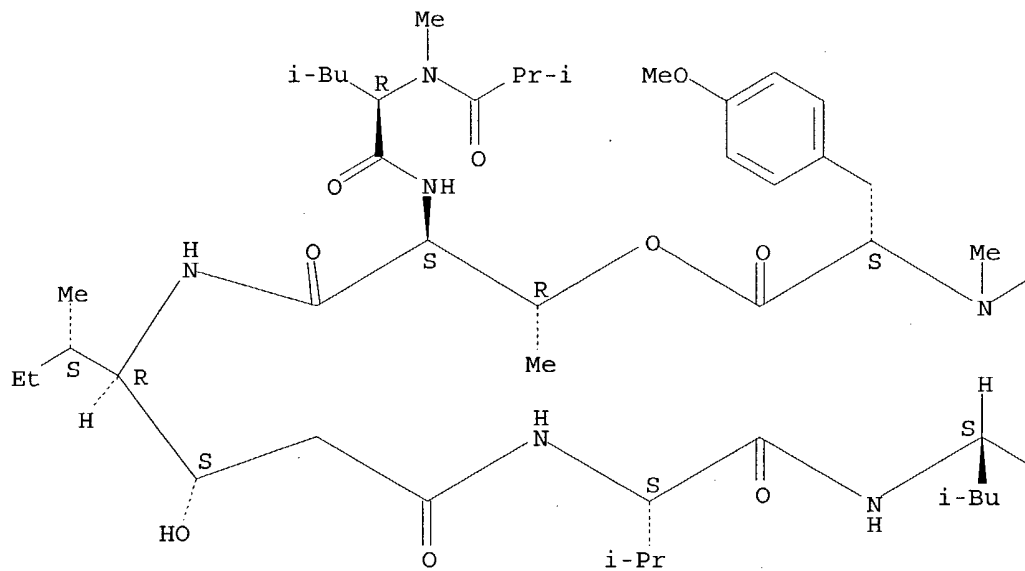
RN 387823-48-5 HCAPLUS

CN L-Tyrosine, N-methyl-N-(2-methyl-1-oxopropyl)-D-leucyl-L-threonyl-  
 (3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-L-valyl-L-leucyl-L-prolyl-  
 N,O-dimethyl-, (7→2)-lactone (9CI) (CA INDEX NAME)

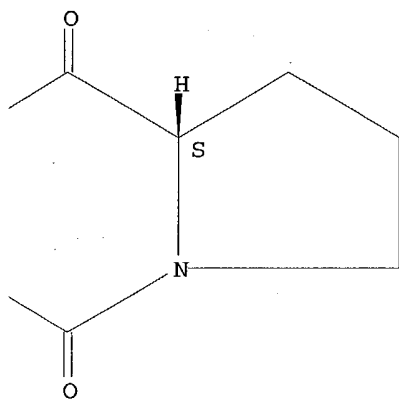
Absolute stereochemistry.

Searched by P. Ruppel

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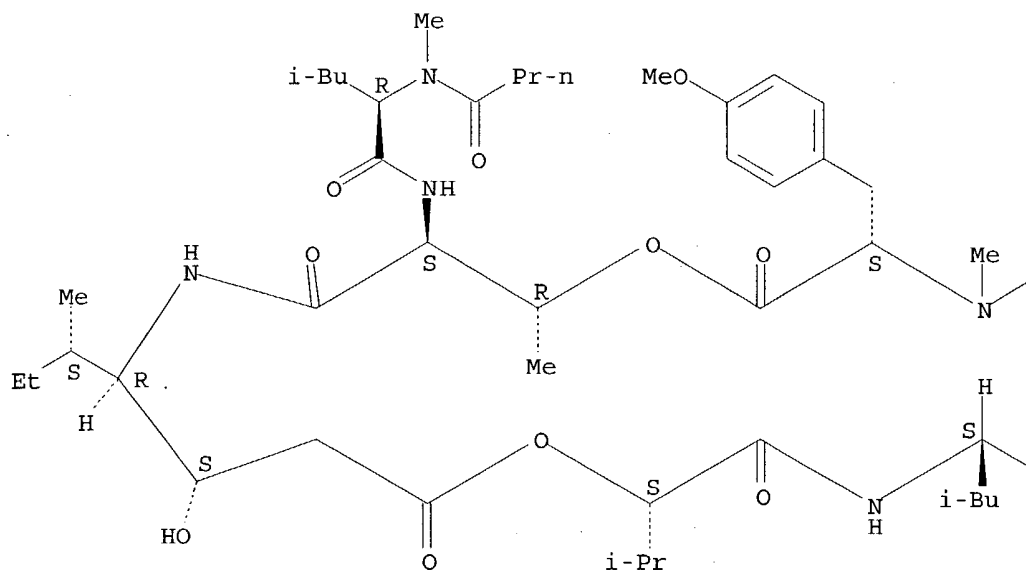
RN 387823-49-6 HCAPLUS

CN L-Tyrosine, N-methyl-N-(1-oxobutyl)-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (7→2)-lactone (9CI) (CA INDEX NAME)

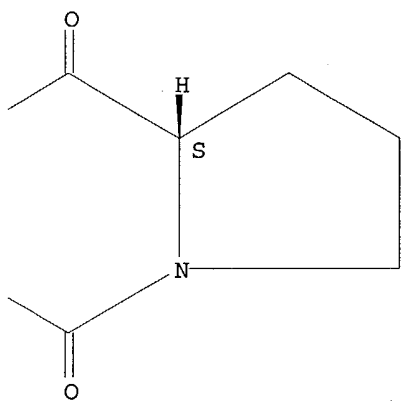
Absolute stereochemistry.

Searched by P. Ruppel

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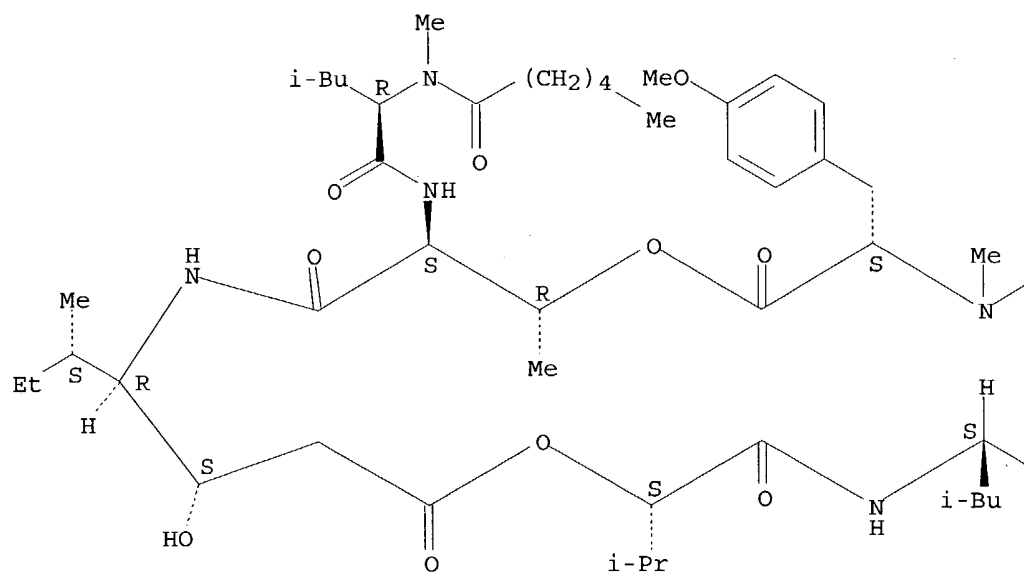
RN 387823-50-9 HCAPLUS

CN L-Tyrosine, N-methyl-N-(1-oxohexyl)-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (7→2)-lactone (9CI) (CA INDEX NAME)

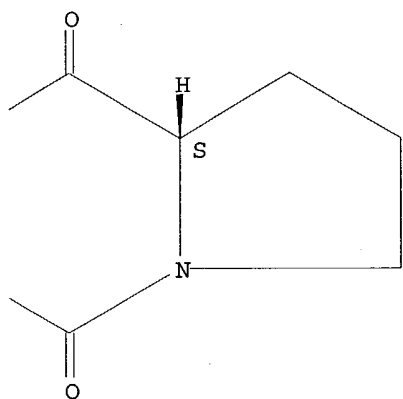
Absolute stereochemistry.

Searched by P. Ruppel

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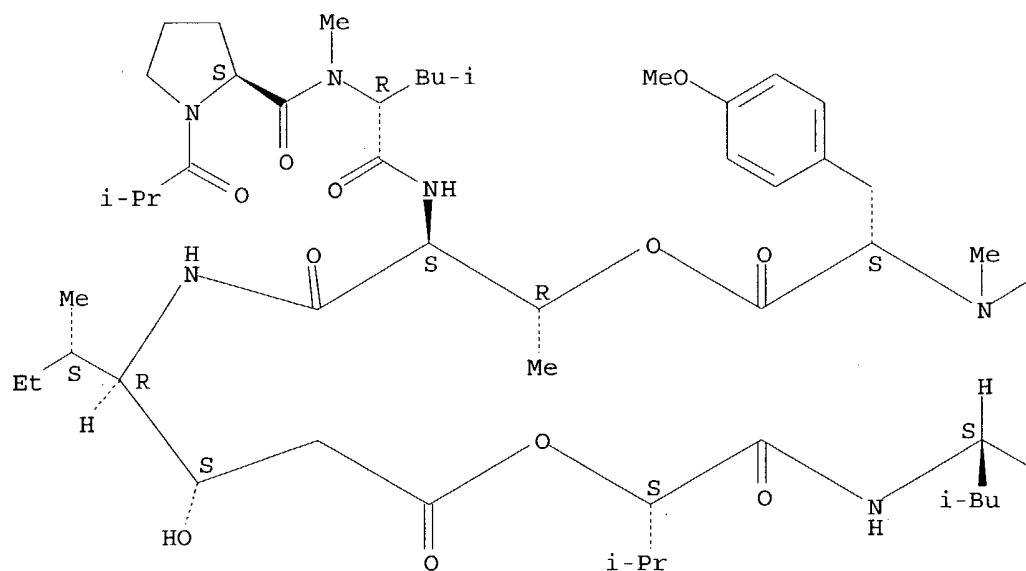


RN 387823-52-1 HCAPLUS  
 CN L-Tyrosine, 1-(2-methyl-1-oxopropyl)-L-prolyl-N-methyl-D-leucyl-L-threonyl-  
 (3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-  
 methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (8→3)-lactone (9CI)  
 (CA INDEX NAME)

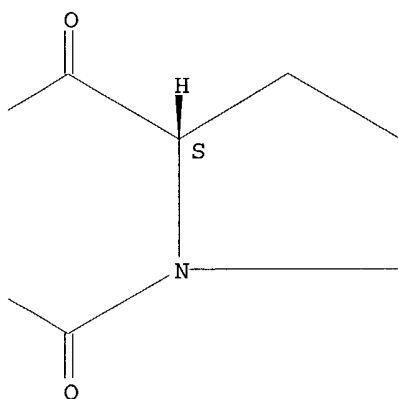
Absolute stereochemistry.

Searched by P. Ruppel

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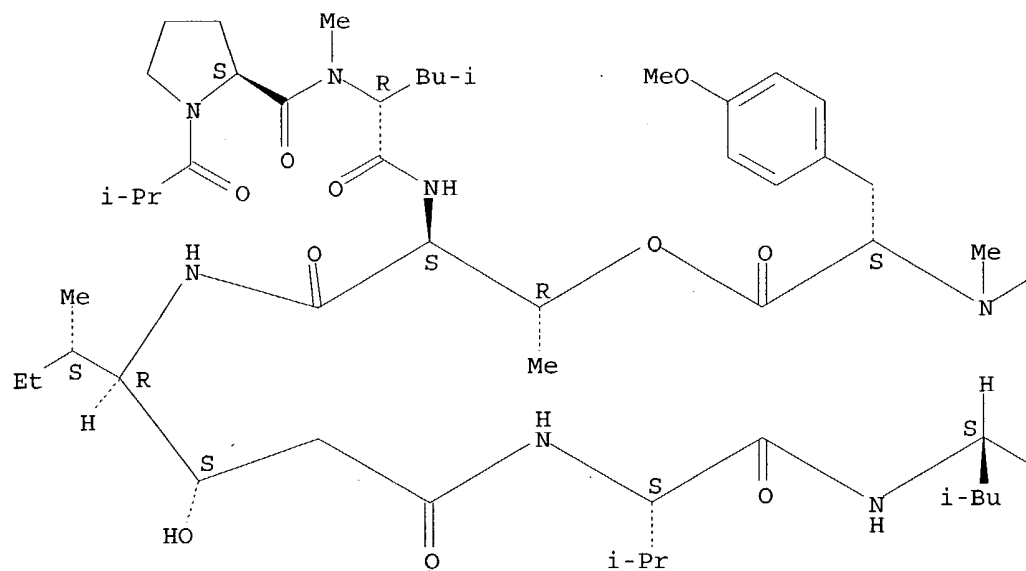
RN 387823-53-2 HCAPLUS

L-Tyrosine, 1-(2-methyl-1-oxopropyl)-L-prolyl-N-methyl-D-leucyl-L-threonyl-  
 (3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-L-valyl-L-leucyl-L-prolyl-  
 N,O-dimethyl-, (8→3)-lactone (9CI) (CA INDEX NAME)

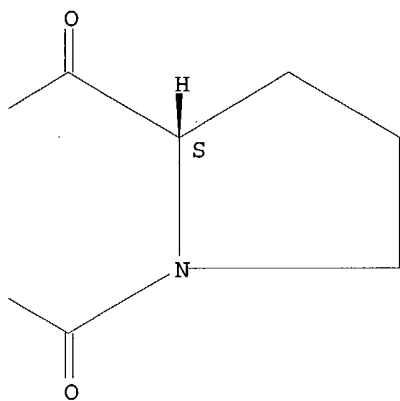
Absolute stereochemistry.

Searched by P. Ruppel

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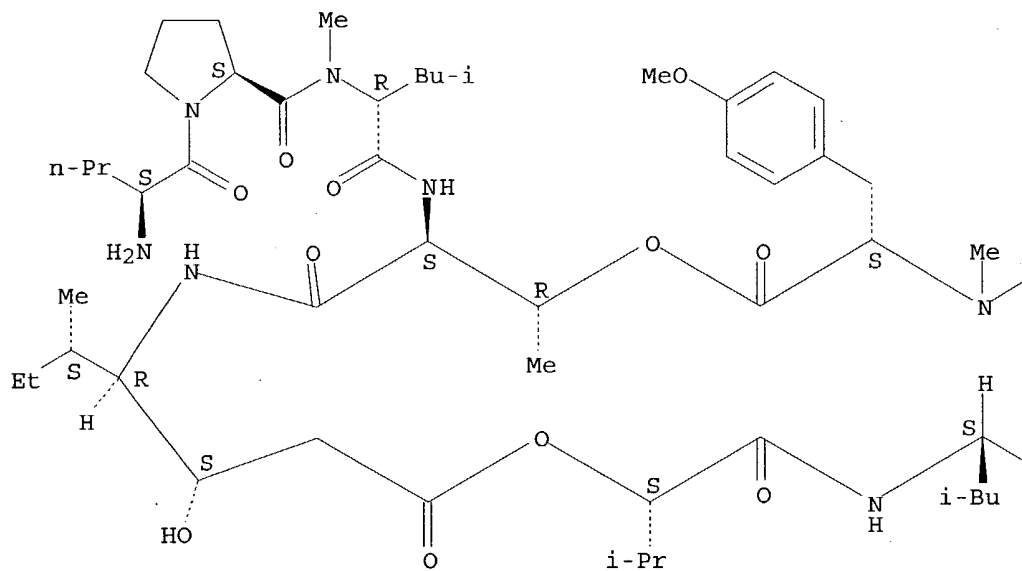
RN 387823-58-7 HCAPLUS

CN L-Tyrosine, L-norvalyl-L-prolyl-N-methyl-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (9→4)-lactone (9CI) (CA INDEX NAME)

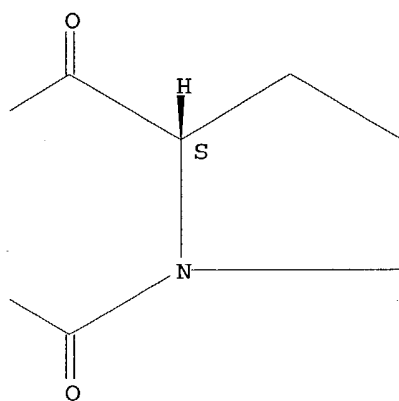
Absolute stereochemistry.

Searched by P. Ruppel

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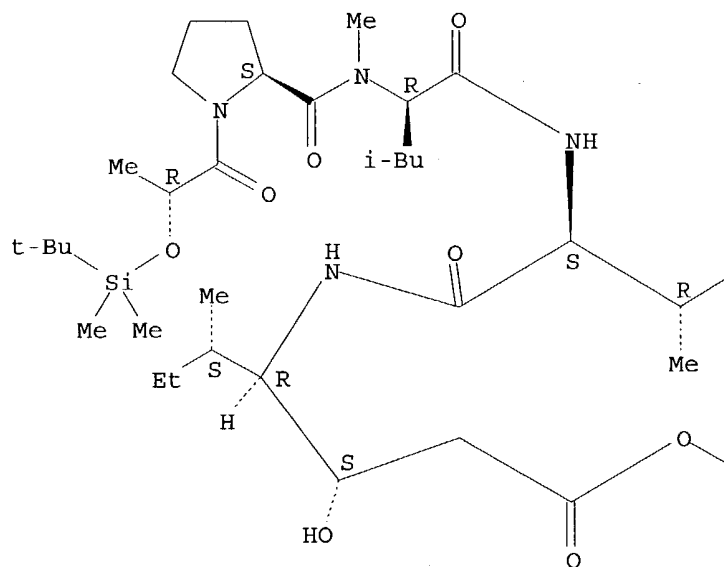
RN 387823-60-1 HCAPLUS

CN L-Tyrosine, 1-[(2R)-2-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1-oxopropyl]-L-prolyl-N-methyl-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (8→3)-lactone (9CI) (CA INDEX NAME)

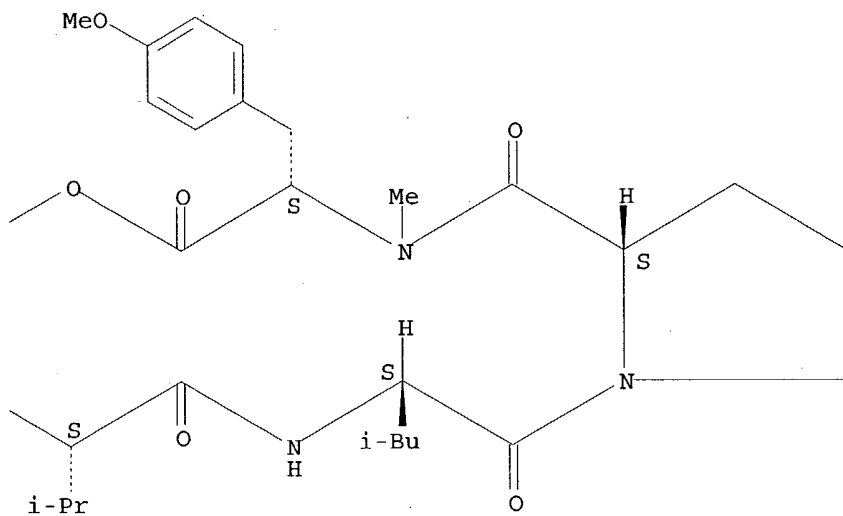
Absolute stereochemistry.

Searched by P. Ruppel

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RN 387823-75-8 HCAPLUS

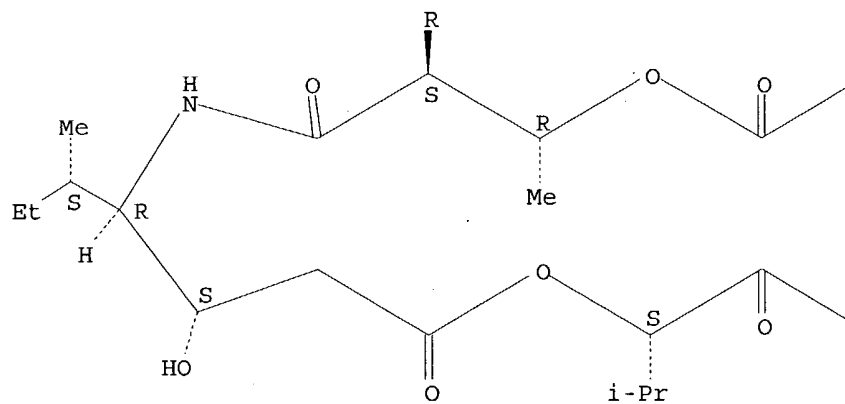
CN L-Tyrosine, N-[(2R)-2-[(5R)-1-[(1,1-dimethylethoxy)carbonyl]-6-oxo-1,7-diazaspiro[4.4]non-7-yl]-4-methyl-1-oxopentyl]-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (6→1)-lactone (9CI) (CA INDEX NAME)

Absolute stereochemistry.

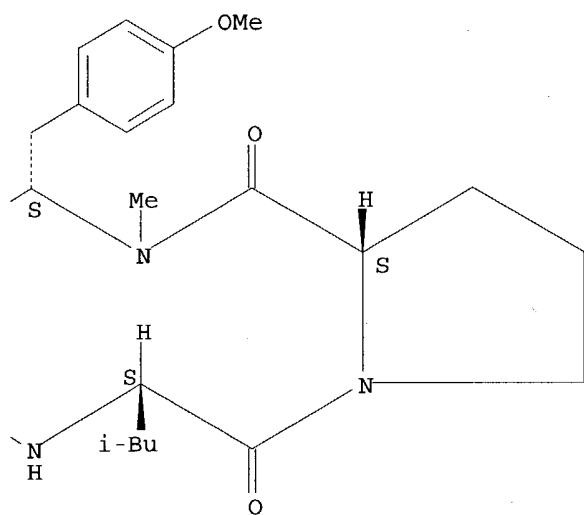
Searched by P. Ruppel



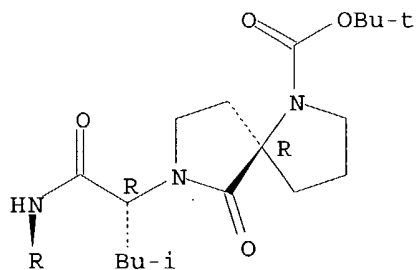
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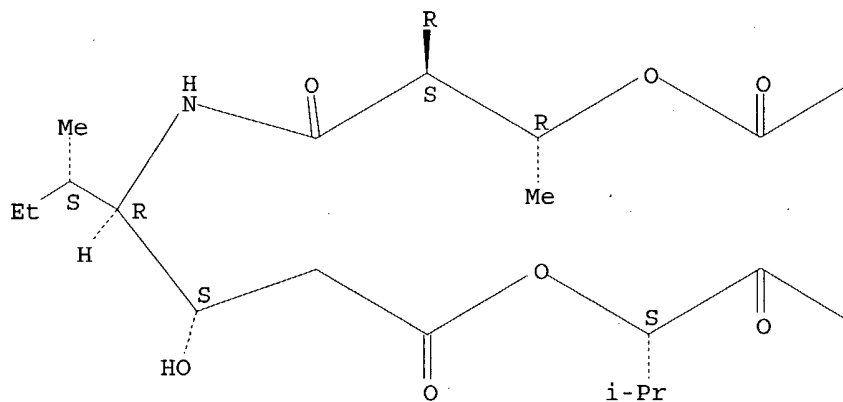


RN 387823-77-0 HCAPLUS

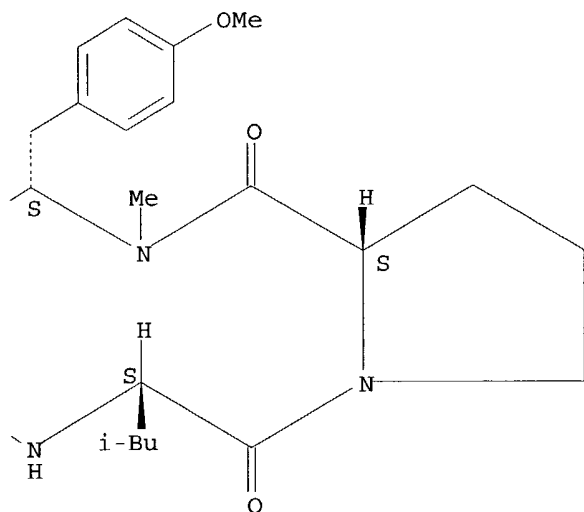
CN L-Tyrosine, N-[(2R)-4-methyl-2-[(5R)-1-(2-methyl-1-oxopropyl)-6-oxo-1,7-diazaspiro[4.4]non-7-yl]-1-oxopentyl]-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (6→1)-lactone (9CI) (CA INDEX NAME)

Absolute stereochemistry.

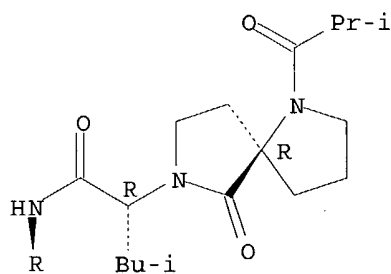
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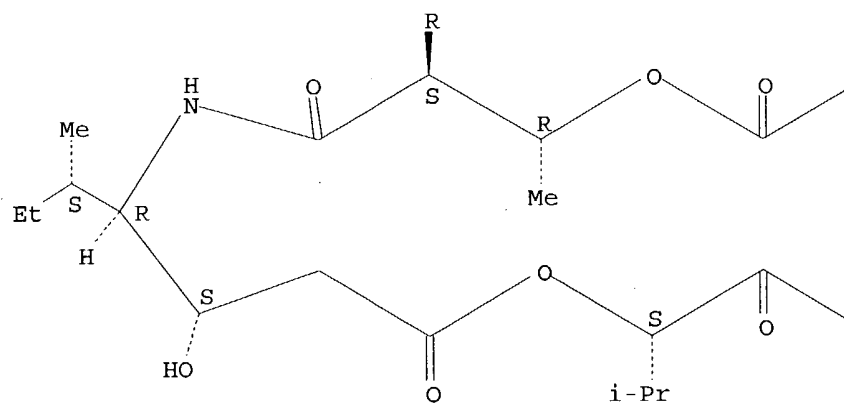


RN 387823-79-2 HCAPLUS

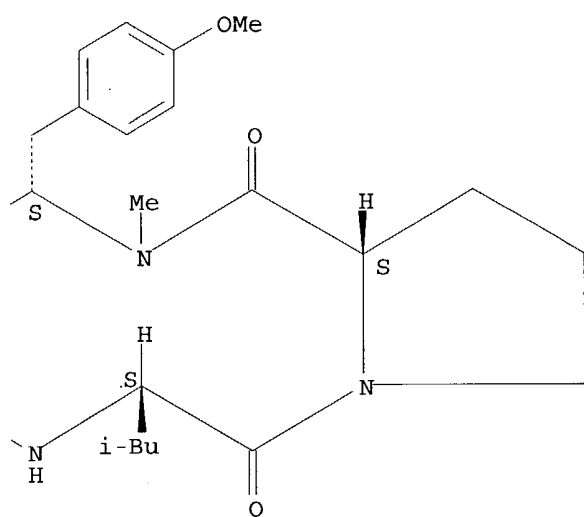
CN L-Tyrosine, N-[(2R)-2-[(5R)-1-(1,2-dioxopropyl)-6-oxo-1,7-diazaspiro[4.4]non-7-yl]-4-methyl-1-oxopentyl]-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (6→1)-lactone (9CI) (CA INDEX NAME)

Absolute stereochemistry.

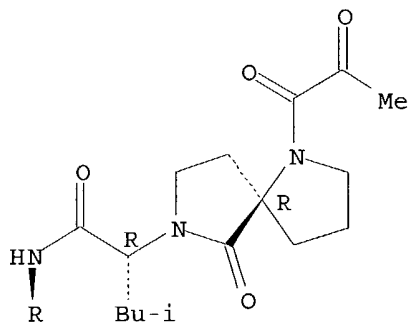
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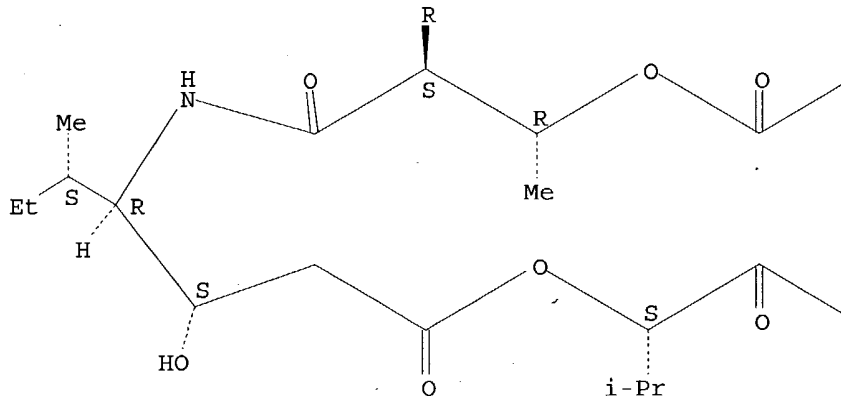


RN 387823-80-5 HCAPLUS

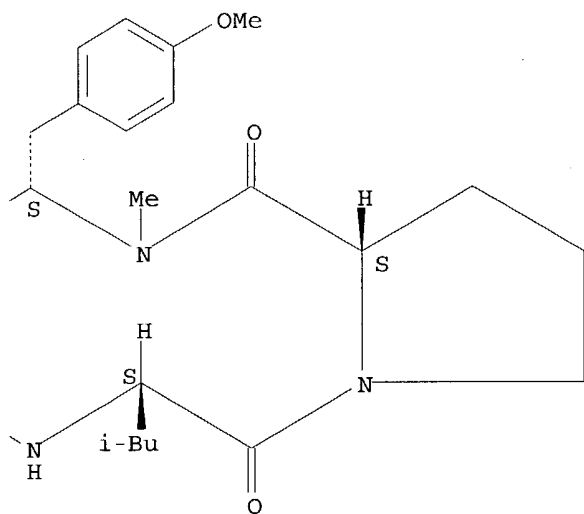
CN L-Tyrosine, N-[(2R)-4-methyl-2-[(5R)-1-(2-methyl-1-oxo-2-propenyl)-6-oxo-1,7-diazaspiro[4.4]non-7-yl]-1-oxopentyl]-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (6→1)-lactone (9CI) (CA INDEX NAME)

Absolute stereochemistry.

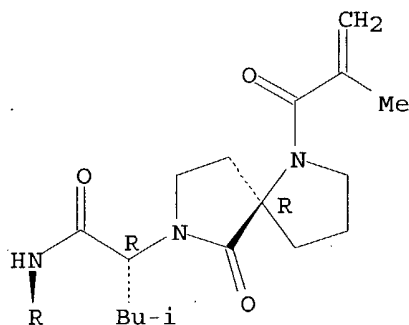
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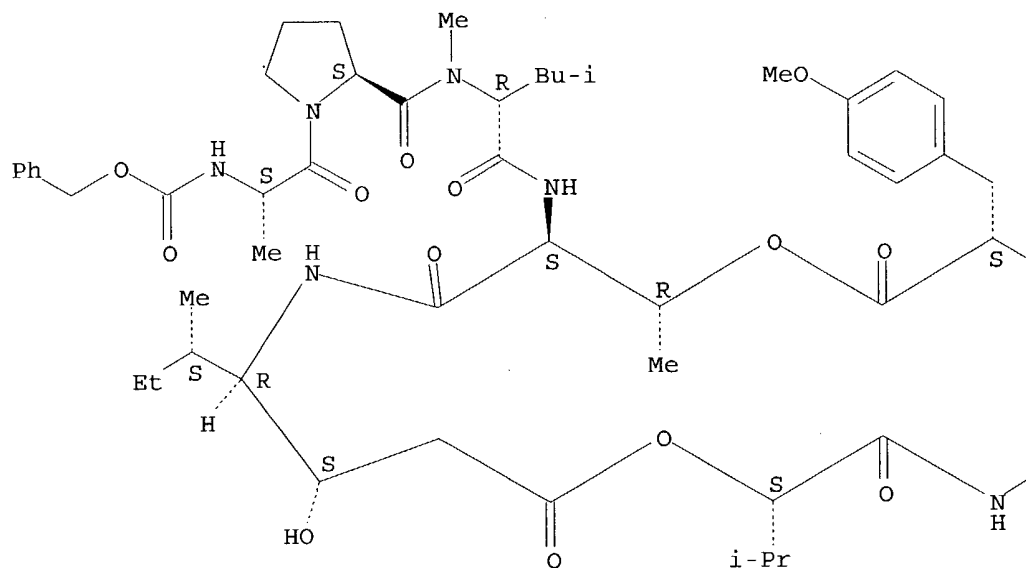


RN 387823-81-6 HCAPLUS

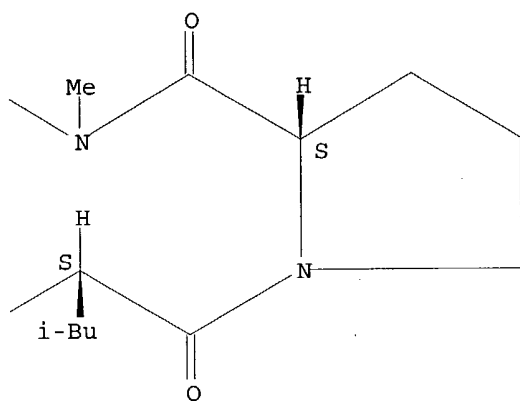
CN L-Tyrosine, N-[(phenylmethoxy)carbonyl]-L-alanyl-L-prolyl-N-methyl-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (9→4)-lactone (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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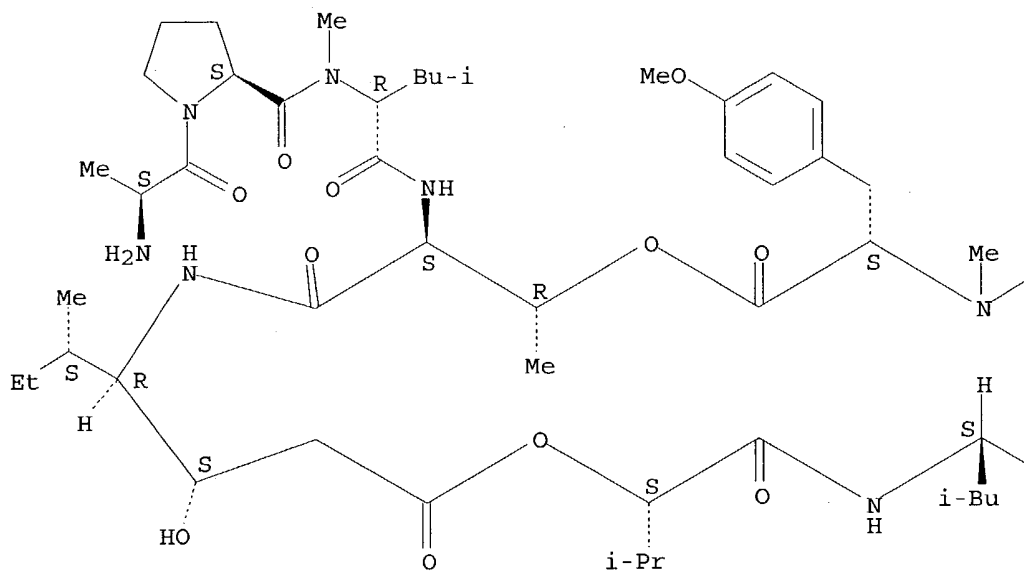
RN 387823-83-8 HCAPLUS

CN L-Tyrosine, L-alanyl-L-prolyl-N-methyl-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (9→4)-lactone, monohydrochloride (9CI) (CA INDEX NAME)

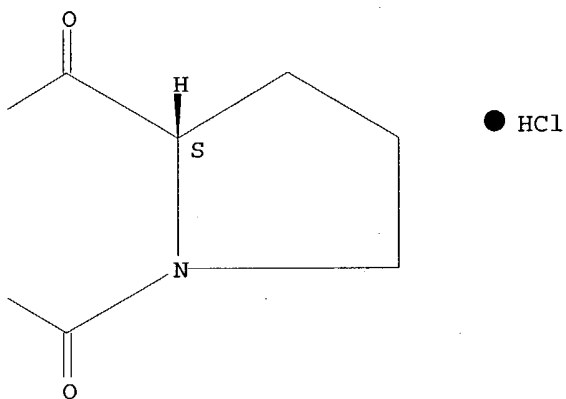
Absolute stereochemistry.

Searched by P. Ruppel

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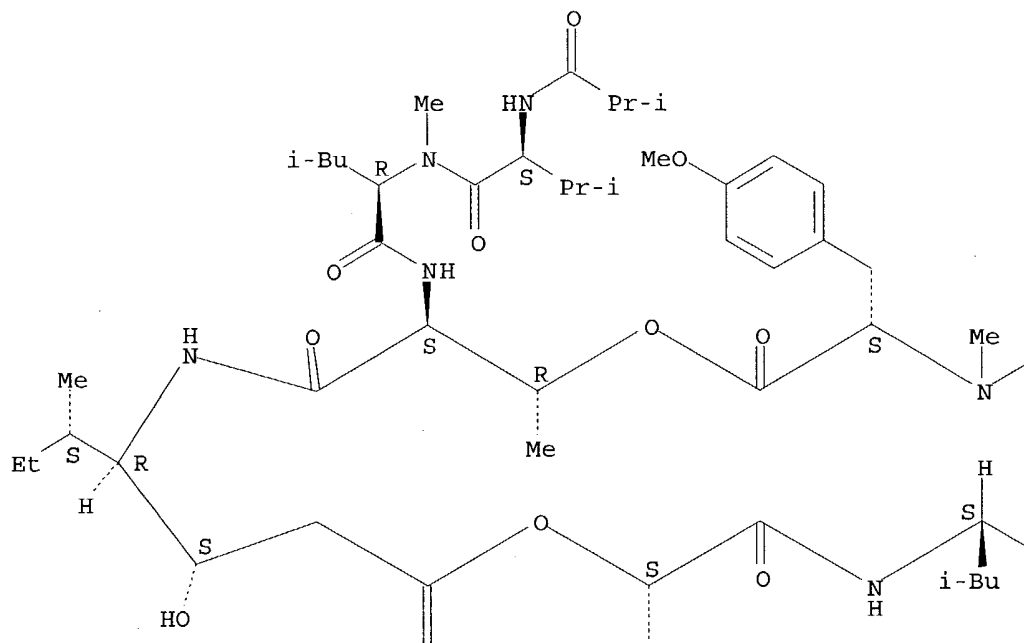
RN 387823-87-2 HCAPLUS  
 CN L-Tyrosine, N-(2-methyl-1-oxopropyl)-L-valyl-N-methyl-D-leucyl-L-threonyl-  
 (3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-  
 methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (8→3)-lactone (9CI)  
 (CA INDEX NAME)

Absolute stereochemistry.

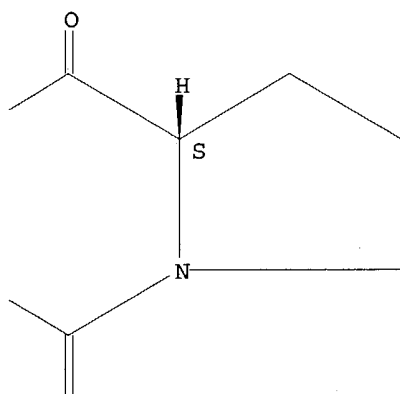
Searched by P. Ruppel



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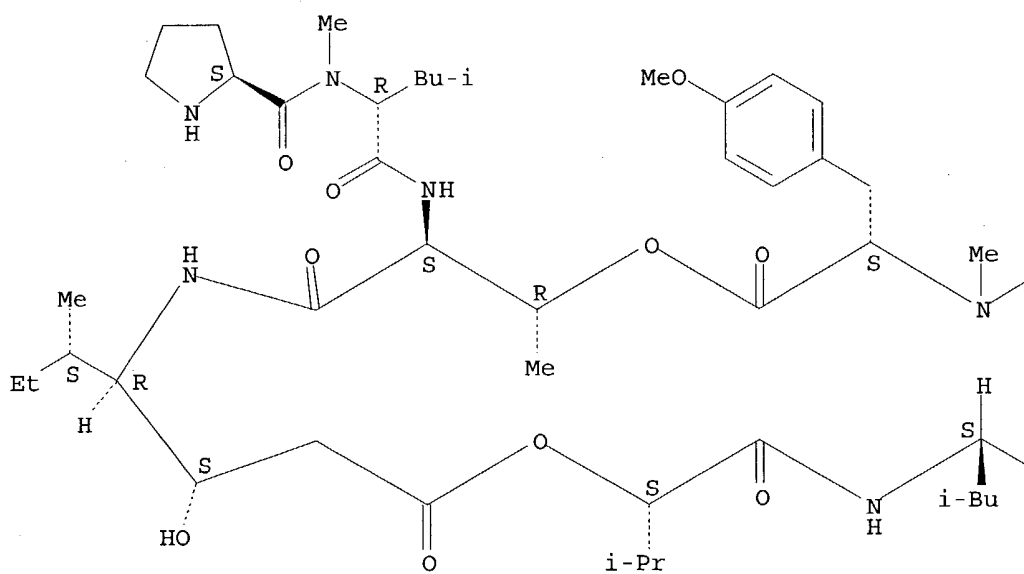
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RN 387859-52-1 HCAPLUS  
 CN L-Tyrosine, L-prolyl-N-methyl-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (8→3)-lactone, monohydrochloride (9CI) (CA INDEX NAME)

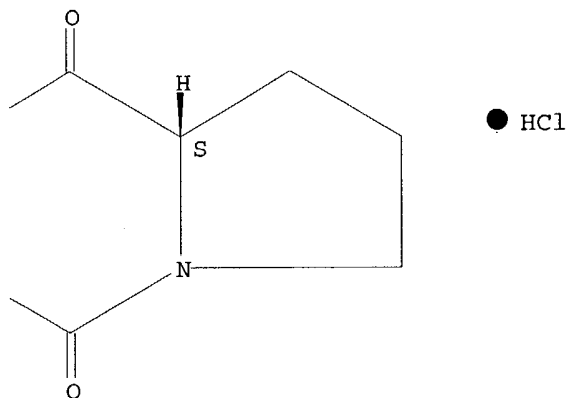
Absolute stereochemistry. Rotation (-).

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Searched by P. Ruppel

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IT 291772-83-3P 387823-38-3P 387823-39-4P  
387823-41-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

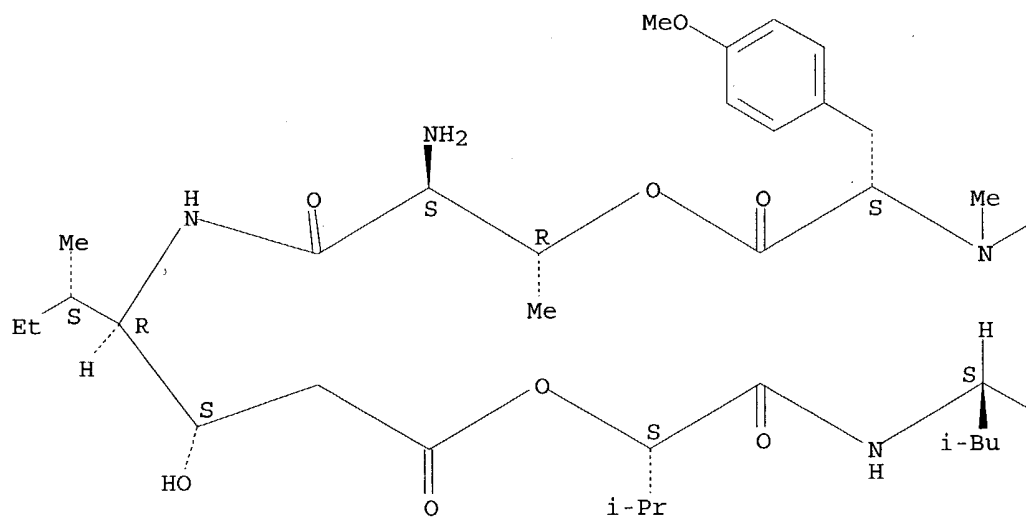
(preparation of aplidine analogs as antitumor agents)

RN 291772-83-3 HCAPLUS

CN L-Tyrosine, L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-  
2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-,  
(6→1)-lactone, monohydrochloride (9CI) (CA INDEX NAME)

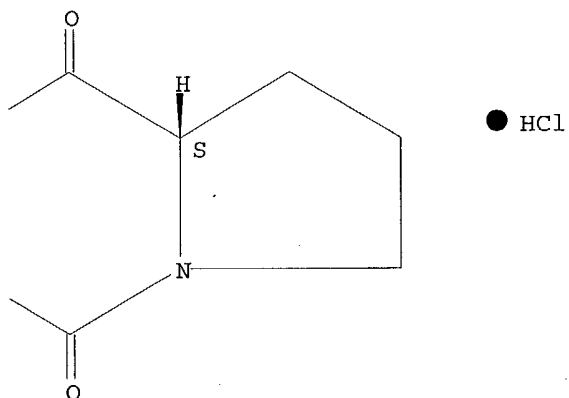
Absolute stereochemistry.

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Searched by P. Ruppel

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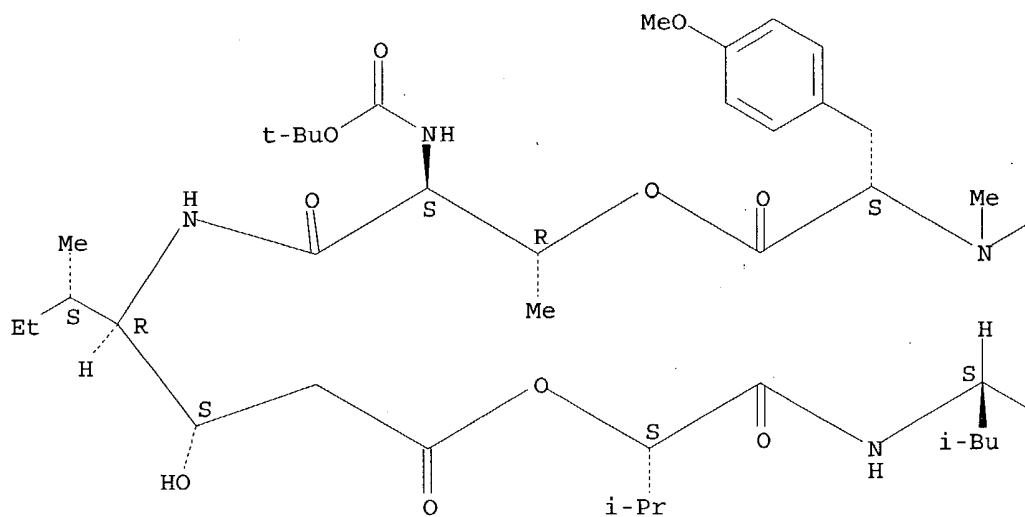


RN 387823-38-3 HCAPLUS

L-Tyrosine, N-[[[1,1-dimethylethoxy)carbonyl]-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (6→1)-lactone (9CI) (CA INDEX NAME)

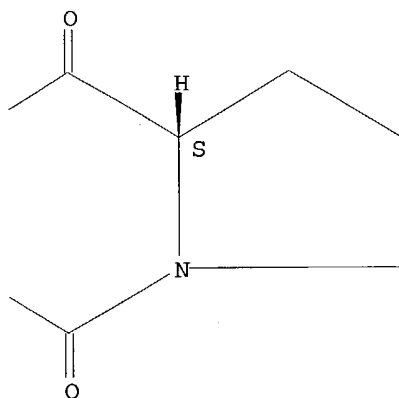
Absolute stereochemistry.

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Searched by P. Ruppel

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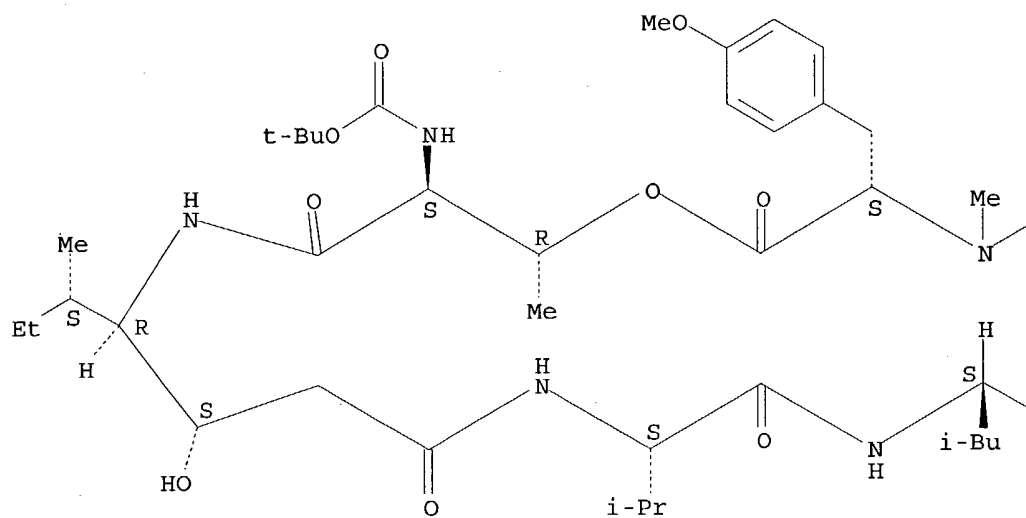


RN 387823-39-4 HCAPLUS

CN L-Tyrosine, N-[(1,1-dimethylethoxy)carbonyl]-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-L-valyl-L-leucyl-L-prolyl-N,O-dimethyl-, (6→1)-lactone (9CI) (CA INDEX NAME)

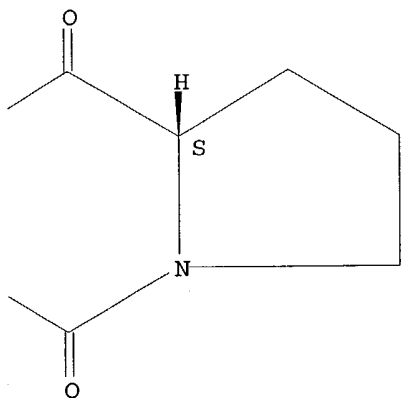
Absolute stereochemistry.

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Searched by P. Ruppel

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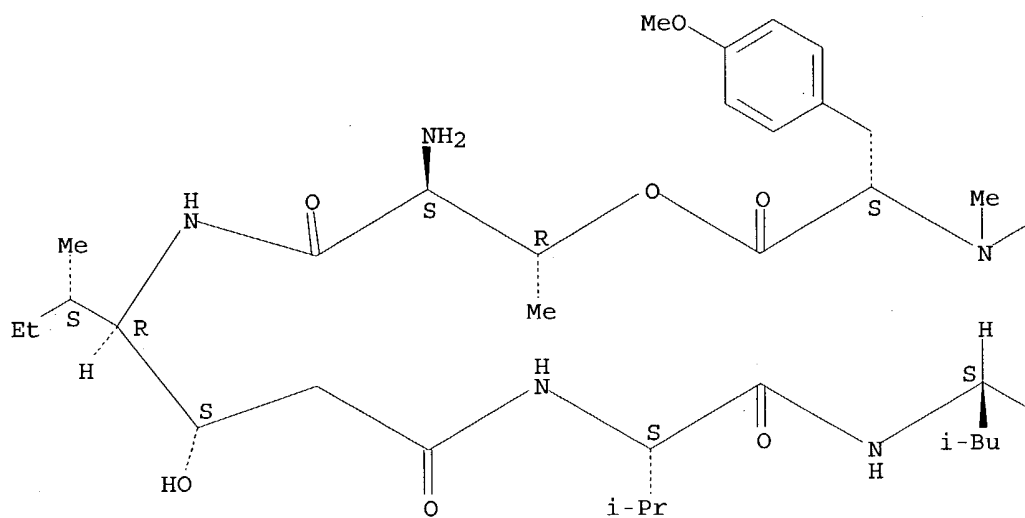


RN 387823-41-8 HCAPLUS

CN L-Tyrosine, L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-L-valyl-L-leucyl-L-prolyl-N,O-dimethyl-, (6→1)-lactone, monohydrochloride (9CI) (CA INDEX NAME)

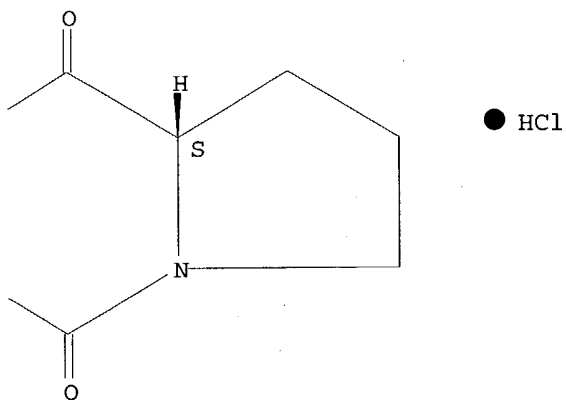
Absolute stereochemistry.

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Searched by P. Ruppel

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L62 ANSWER 3 OF 10 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:16567 HCAPLUS

DOCUMENT NUMBER: 137:140752

TITLE: Part I. Total synthesis and biological investigations of tamandarin compounds. Part II. Synthetic studies towards the total synthesis of callipeltin A

AUTHOR(S): Liang, Bo

CORPORATE SOURCE: Univ. of Pennsylvania, Philadelphia, PA, USA

SOURCE: (2001) 455 pp. Avail.: UMI, Order No. DA3003653  
From: Diss. Abstr. Int., B 2001, 62(2), 864

DOCUMENT TYPE: Dissertation

LANGUAGE: English

AB Unavailable

IT 250211-78-0P, Tamandarin A

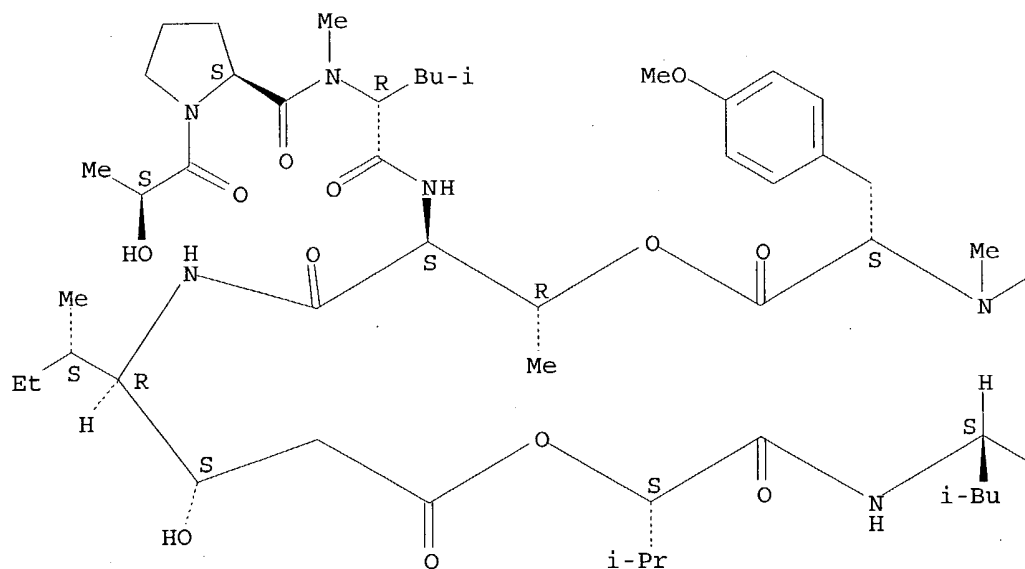
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL  
(Biological study); PREP (Preparation)  
(total synthesis and biol. investigations of tamandarin compds.)

RN 250211-78-0 HCAPLUS

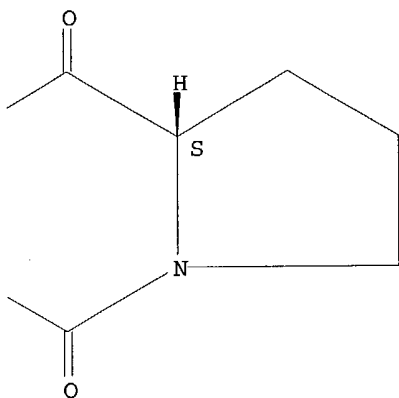
CN Tamandarin A (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

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L62 ANSWER 4 OF 10 HCAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 2001:762837 HCAPLUS  
DOCUMENT NUMBER: 135:318713  
TITLE: Preparation of tamandarin and didemnin analogs  
INVENTOR(S): J  ullie, Madeleine M.; Liang, Bo; Ding, Xiaobin  
PATENT ASSIGNEE(S): Trustees of the University of Pennsylvania, USA  
SOURCE: PCT Int. Appl., 190 pp.

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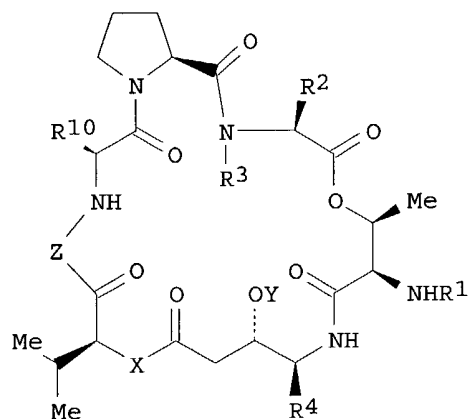


CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001076616	A1	20011018	WO 2001-US11607	20010409
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6509315	B1	20030121	US 2000-545848	20000407
US 2001056178	A1	20011227	US 2001-767080	20010122
EP 1276491	A1	20030122	EP 2001-924886	20010409
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2001009958	A	20030527	BR 2001-9958	20010409
JP 2003535048	T2	20031125	JP 2001-574132	20010409
PRIORITY APPLN. INFO.:				
			US 2000-545848	A 20000407
			US 2001-767080	A 20010122
			WO 2001-US11607	W 20010409

OTHER SOURCE(S): CASREACT 135:318713; MARPAT 135:318713

GI



AB The invention relates to tamandarin and didemnin analogs I (Z = null or COCHMe, resp.; R1 = H, tert-butoxycarbonyl, leucyl, N-methyllleucyl, a residue having a deoxoproline or dehydroproline residue, etc.; R2 is an isoleucine, valine, alanine, norleucine, norvaline, leucine, histidine, tryptophan, arginine or lysine side chain or a substituted benzyl group; R3 = H, Me or R2R3 is a substituted o-phenylenemethylene group; R4 is an isoleucine or valine side chain; X = O or NH; Y = H or a hydroxy-protecting group) which are useful as anticancer agents, inhibitors of protein synthesis, cell growth and tumorigenesis and as enhancers of apoptosis. (-)-Tamandarin A is not claimed but a total

synthesis was carried out. The synthesis of a didemnin B analog in which R1 is 3,4-dehydro-L-prolyl-N-methyl-D-leucyl is described.

IT 250211-78-0P, Tamandarin a 258339-38-7P, Tamandarin B

291772-81-1P, Tamandarin M 345969-81-5P

367507-41-3P 367507-42-4P 367507-44-6P

367507-45-7P 367507-46-8P 367507-47-9P

367507-48-0P 367507-49-1P 367507-50-4P

367507-51-5P 367507-52-6P 367507-53-7P

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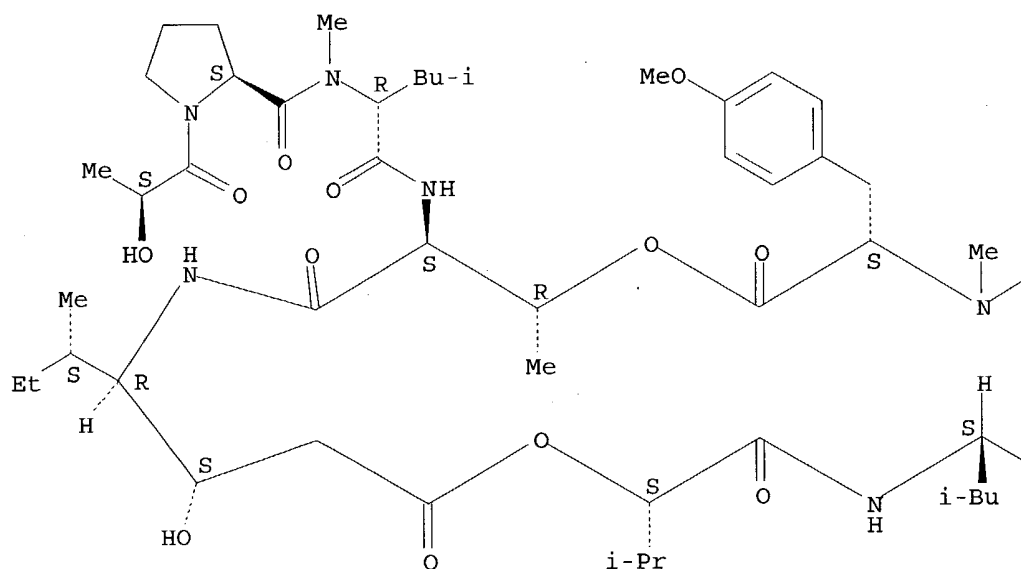
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of tamandarin and didemnin analogs)

RN 250211-78-0 HCAPLUS

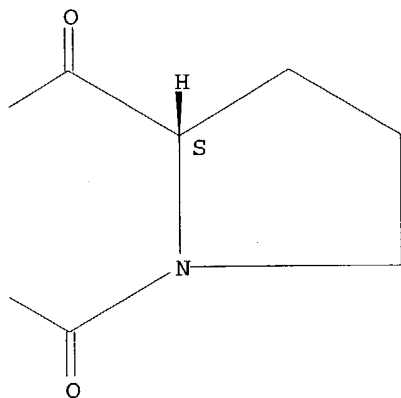
CN Tamandarin A (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

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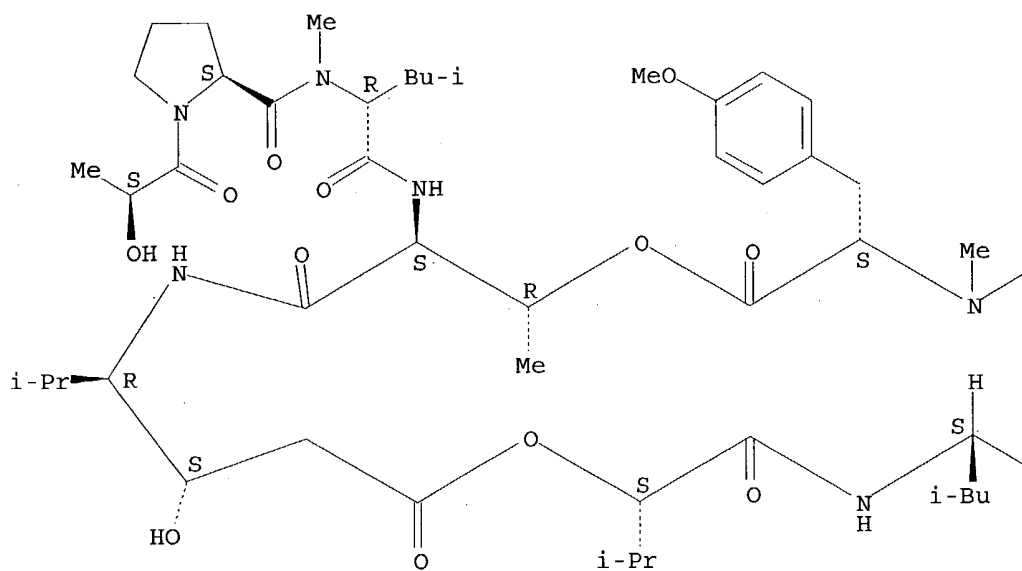
PAGE 1-B



RN 258339-38-7 HCAPLUS  
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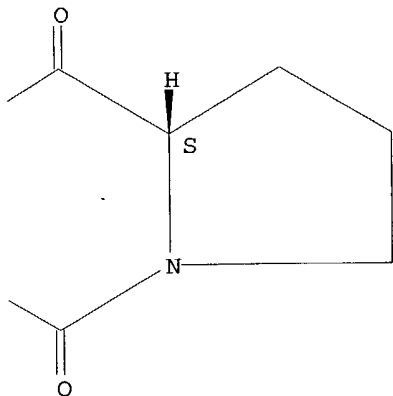
Absolute stereochemistry. Rotation (-).

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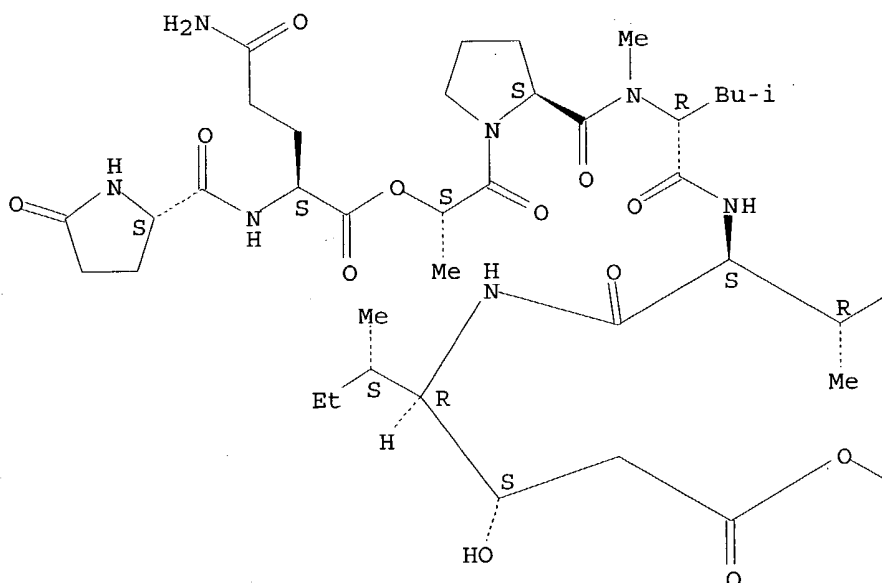
PAGE 1-B



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NAME)

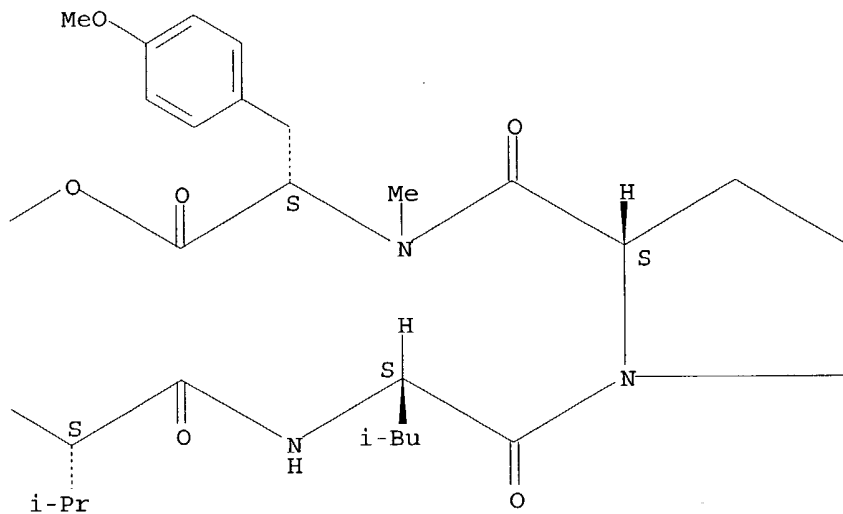
Absolute stereochemistry. Rotation (-).

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Searched by P. Ruppel

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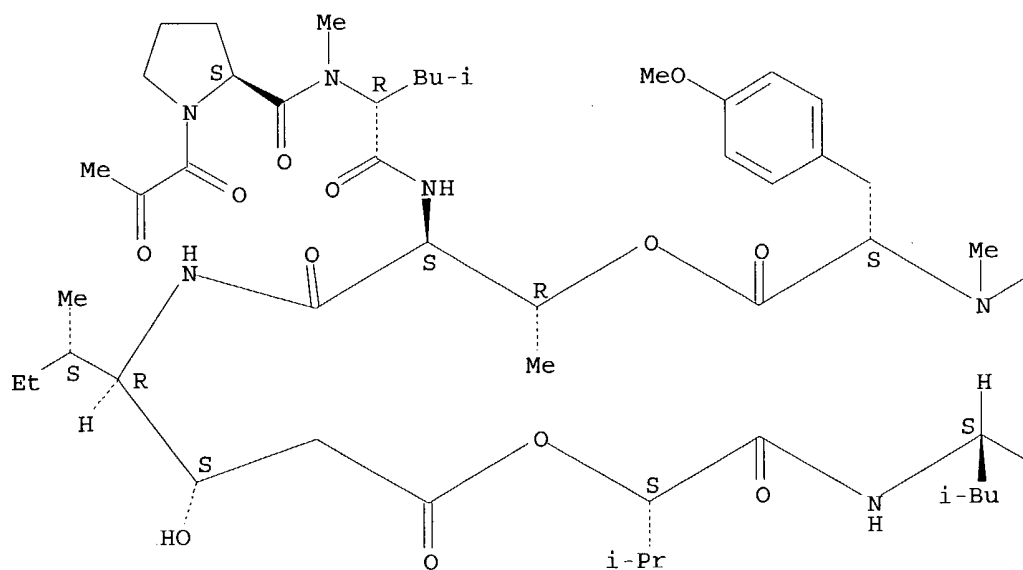


RN 345969-81-5 HCAPLUS

CN L-Tyrosine, 1-(1,2-dioxopropyl)-L-prolyl-N-methyl-D-leucyl-L-threonyl-  
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 (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

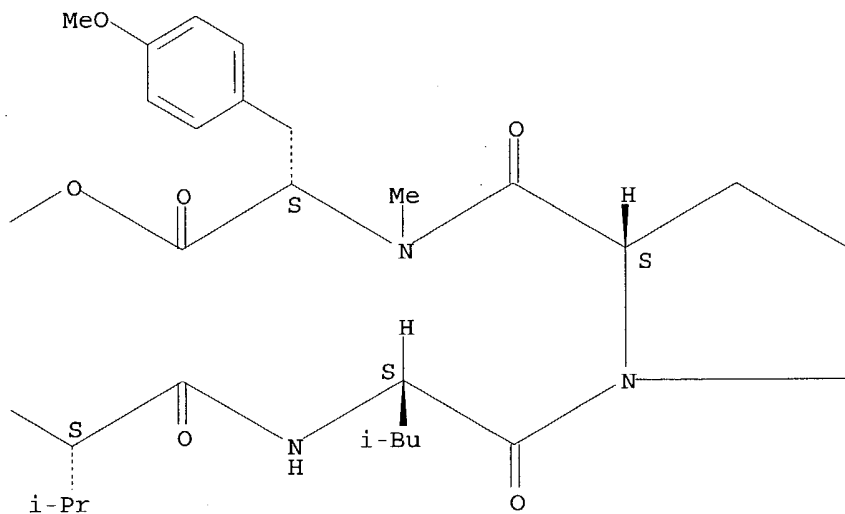
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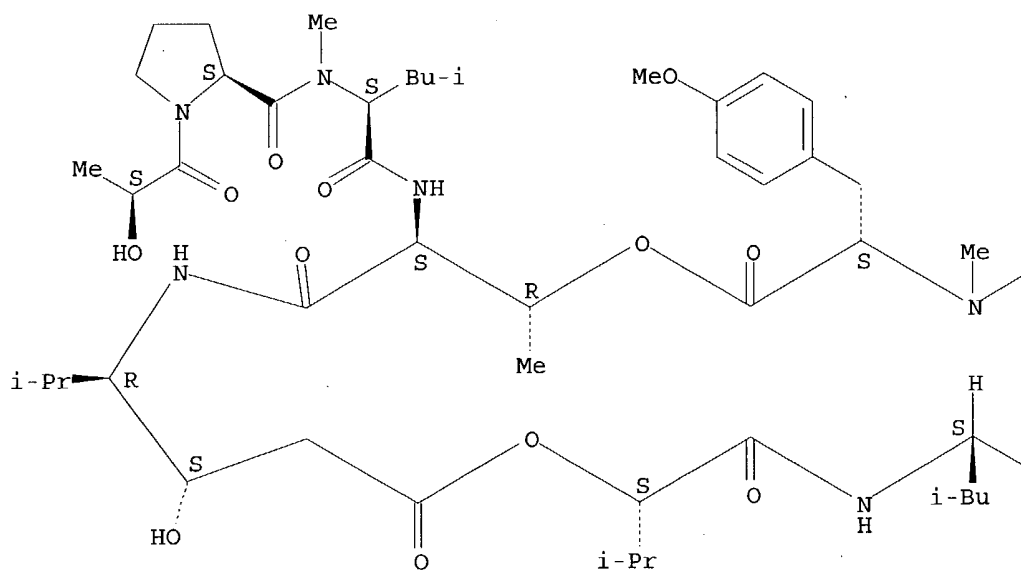


RN 367507-42-4 HCAPLUS

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 NAME)

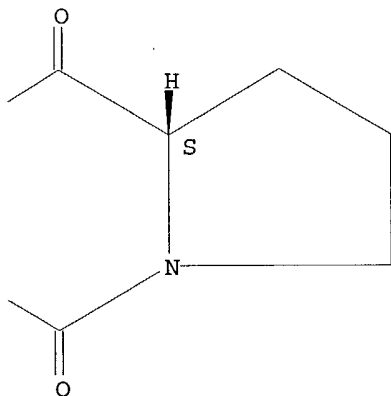
Absolute stereochemistry.

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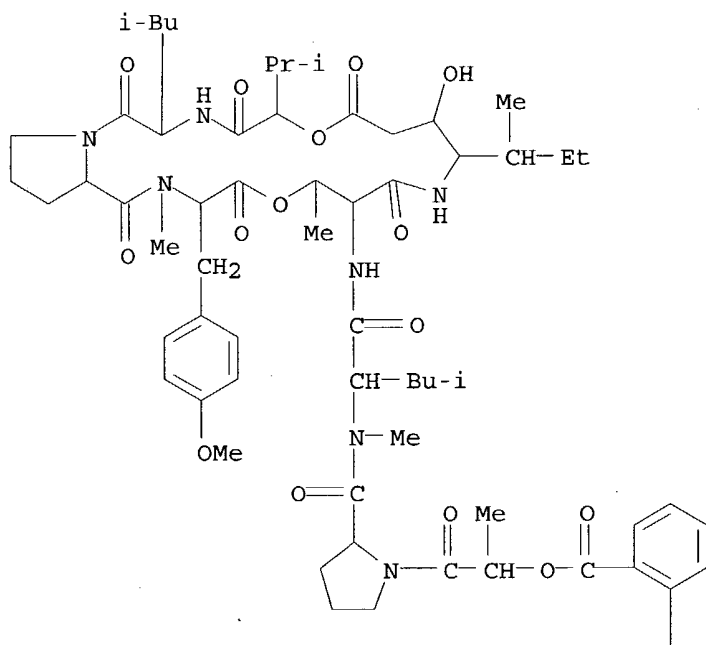
Searched by P. Ruppel

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RN 367507-44-6 HCAPLUS  
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(CA INDEX NAME)

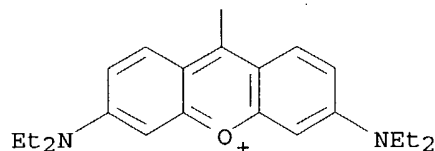
PAGE 1-A



Searched by P. Ruppel

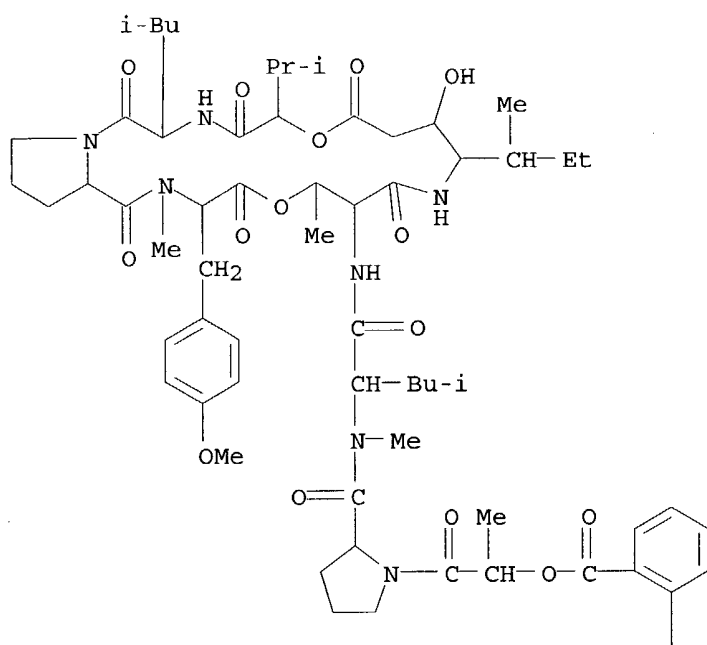


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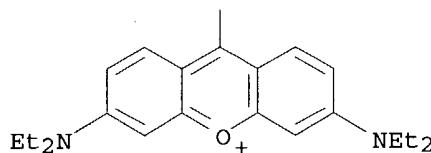


RN 367507-45-7 HCAPLUS  
 CN Tamandarin A, 3-(N-methyl-L-leucine)-, 1-[2-[3,6-bis(diethylamino)xanthylum-9-yl]benzoate] (9CI) (CA INDEX NAME)

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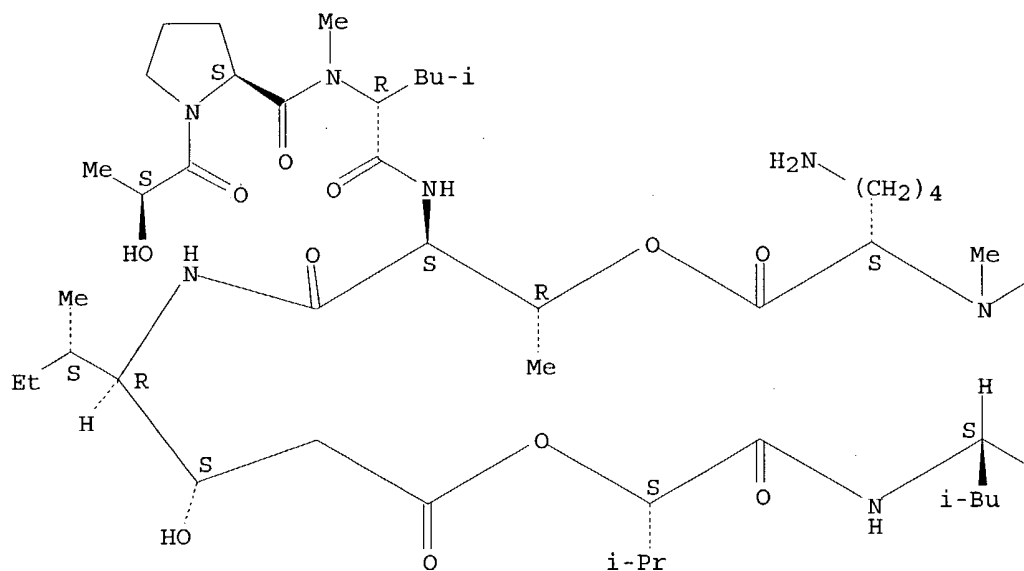


RN 367507-46-8 HCAPLUS  
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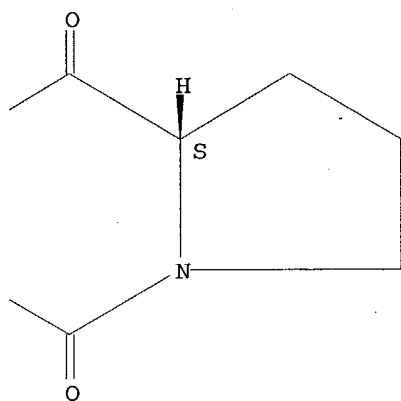
Absolute stereochemistry.

Searched by P. Ruppel

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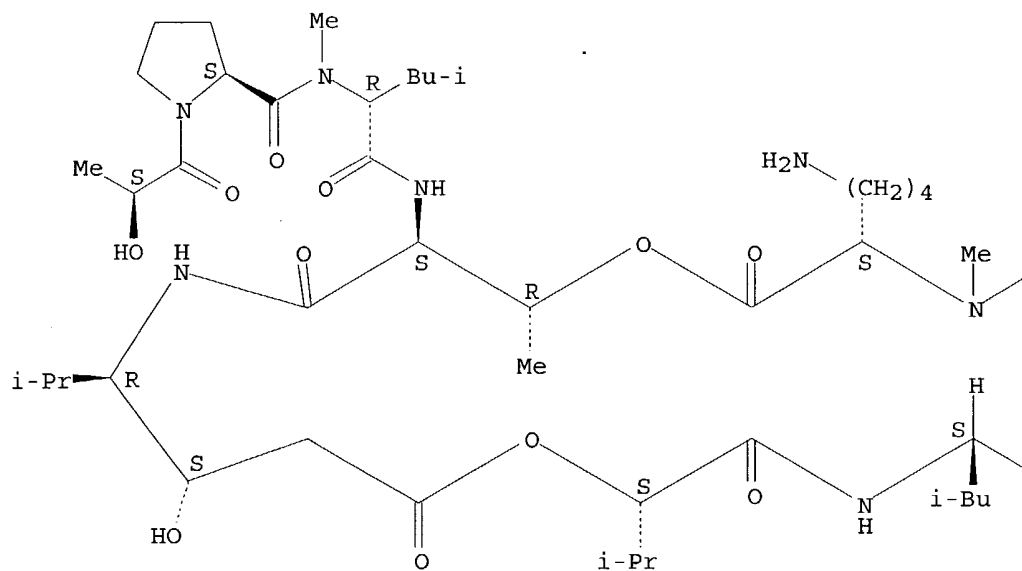
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 (3S,4R)-4-amino-3-hydroxy-5-methylhexanoyl-(2S)-2-hydroxy-3-methylbutanoyl-  
 L-leucyl-L-prolyl-N2-methyl-, (9→4)-lactone (9CI) (CA INDEX NAME)

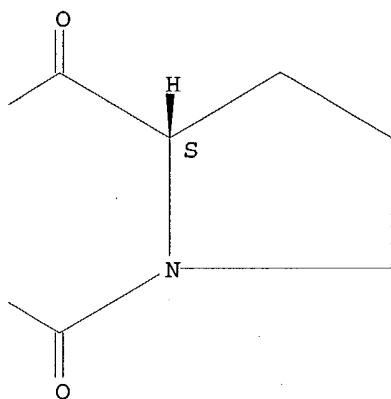
Absolute stereochemistry.

Searched by P. Ruppel

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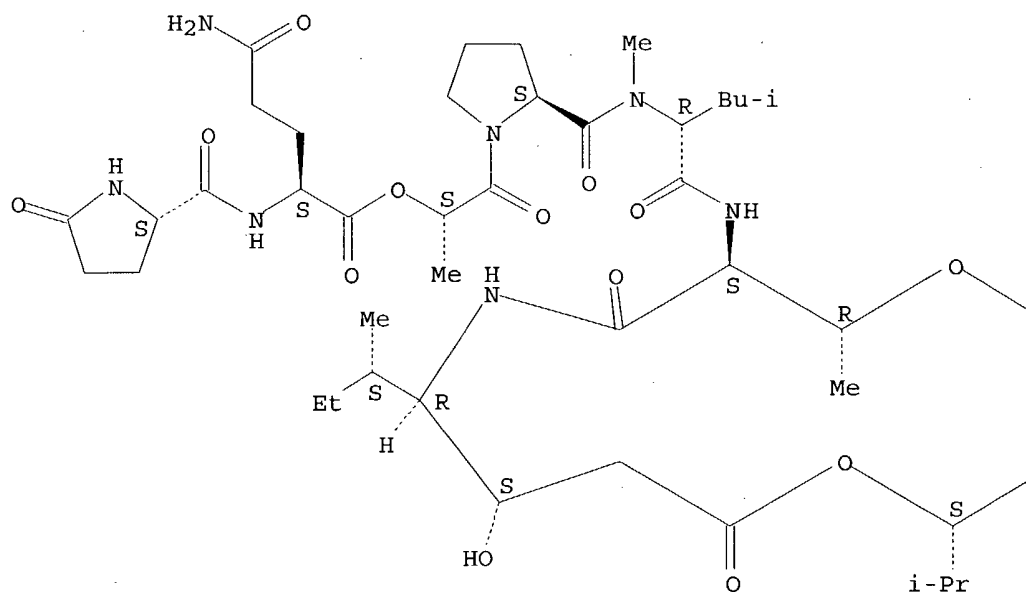
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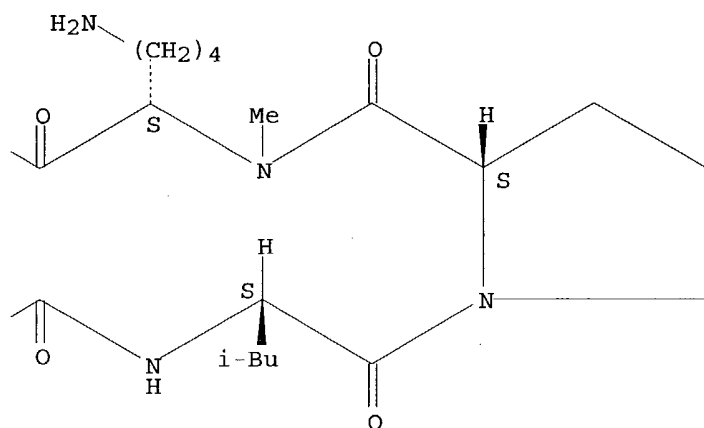
Absolute stereochemistry.

Searched by P. Ruppel

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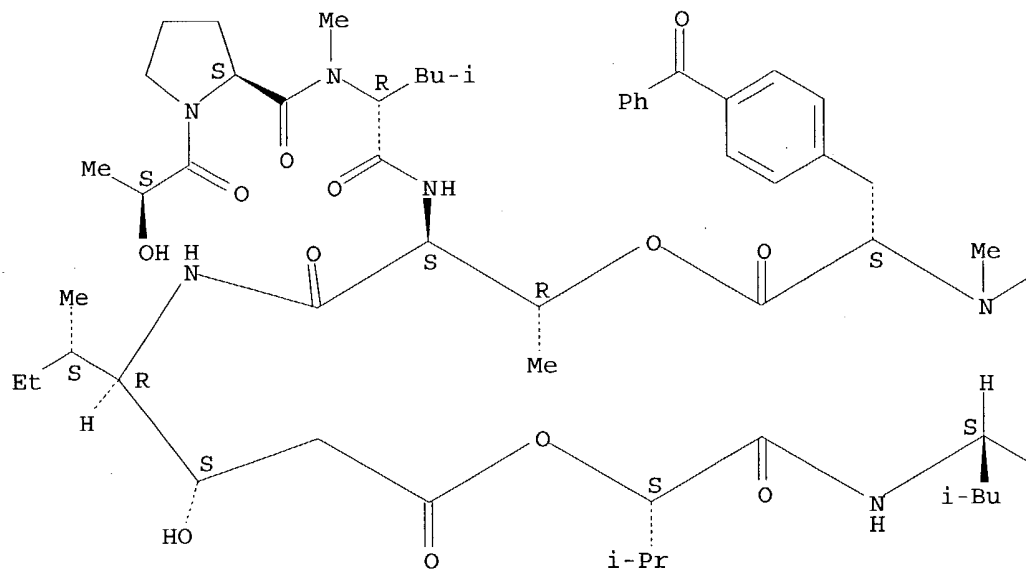
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CN L-Phenylalanine, (2S)-2-hydroxypropanoyl-L-prolyl-N-methyl-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-4-benzoyl-N-methyl-, (9→4)-lactone  
(9CI) (CA INDEX NAME)

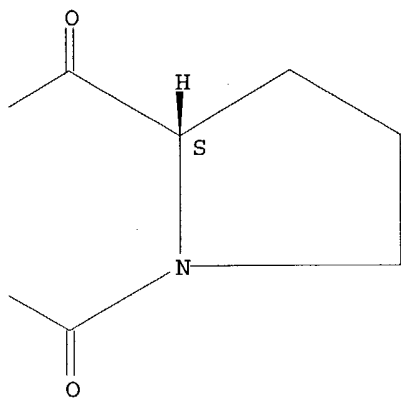
Absolute stereochemistry.

Searched by P. Ruppel

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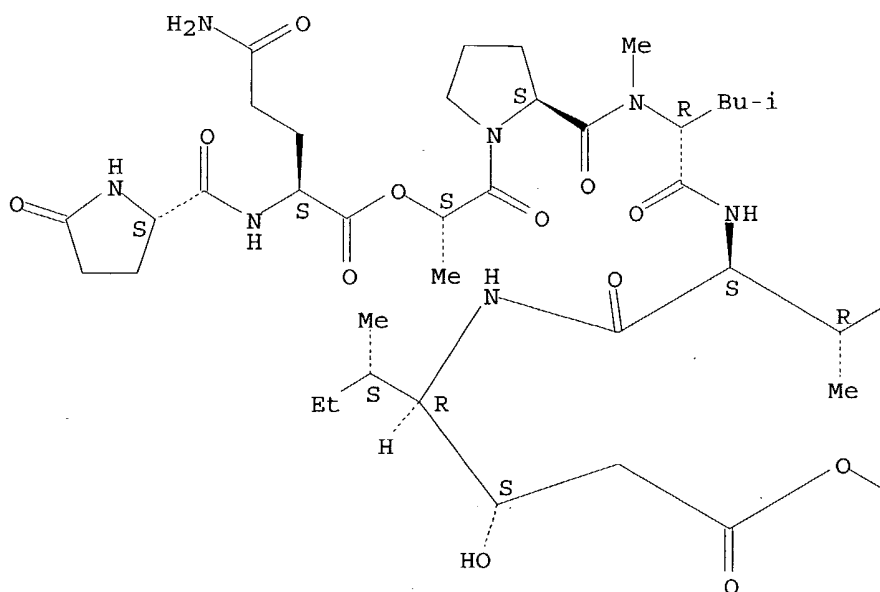
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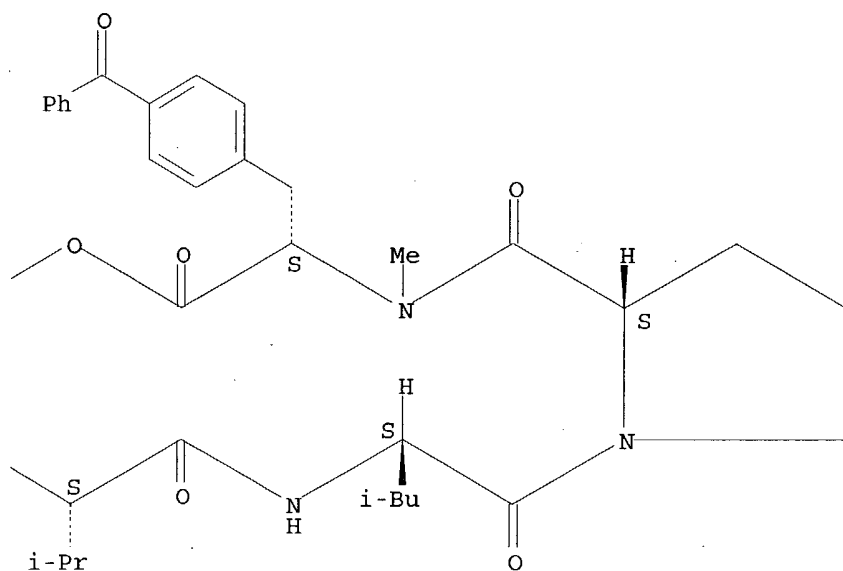
Absolute stereochemistry.

Searched by P. Ruppel

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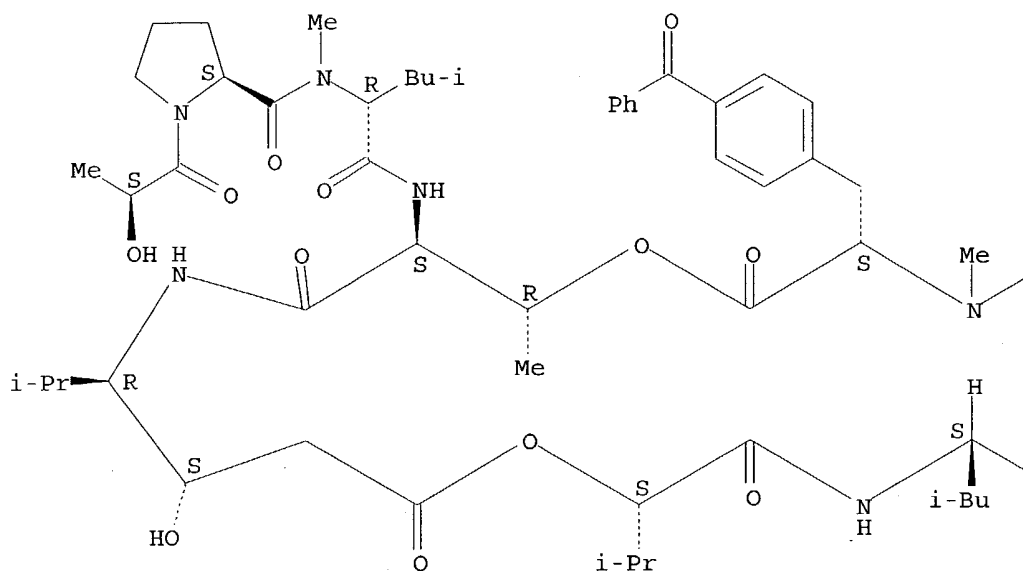
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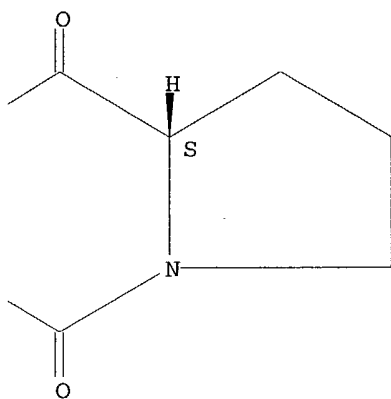
Absolute stereochemistry.

Searched by P. Ruppel

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RN 367507-52-6 HCAPLUS  
 CN Tamandarin A, 9-[(3S)-1,2,3,4-tetrahydro-7-methoxy-3-isoquinolinecarboxylic acid]- (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 367507-53-7 HCAPLUS  
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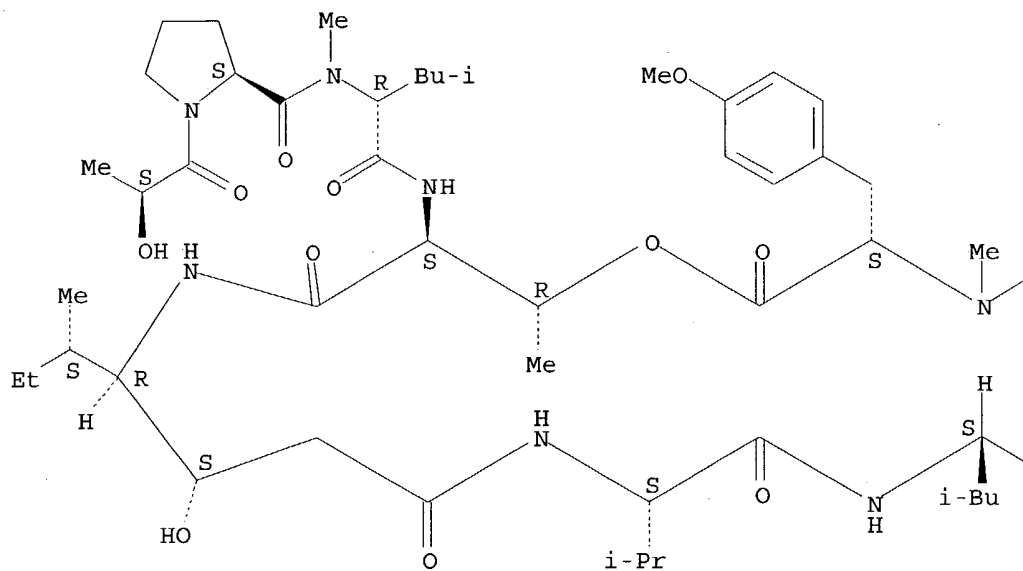
\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

CN Tamandarin B, 9-[(3S)-1,2,3,4-tetrahydro-7-methoxy-3-isoquinolinecarboxylic acid]-(9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

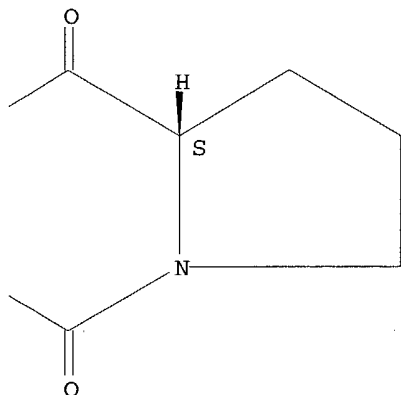
CN Tamandarin A, 6-L-valine- (9CI) (CA INDEX NAME)

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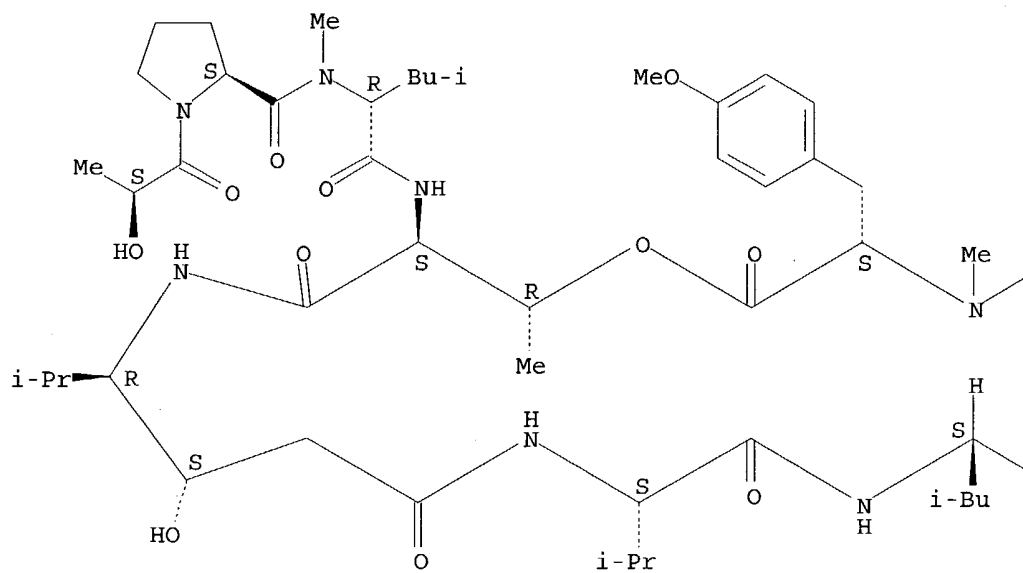
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RN 367507-56-0 HCAPLUS  
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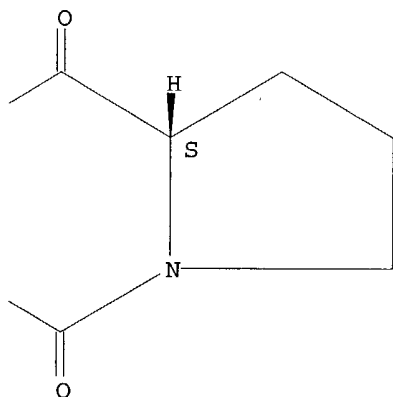
Absolute stereochemistry.

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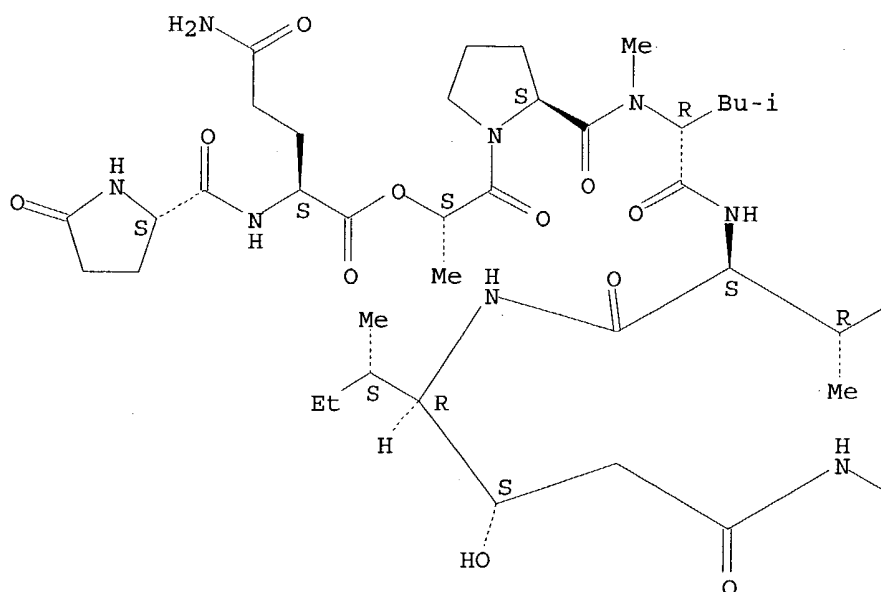


RN 367507-57-1 HCAPLUS

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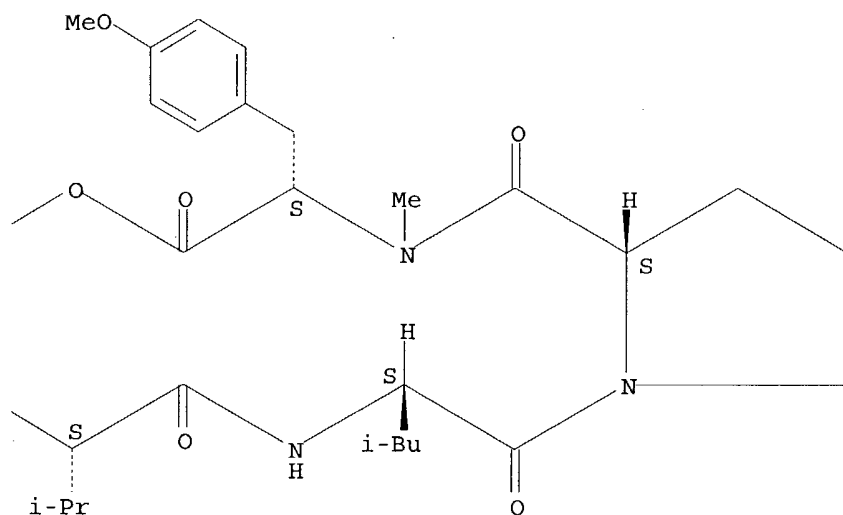
Absolute stereochemistry.

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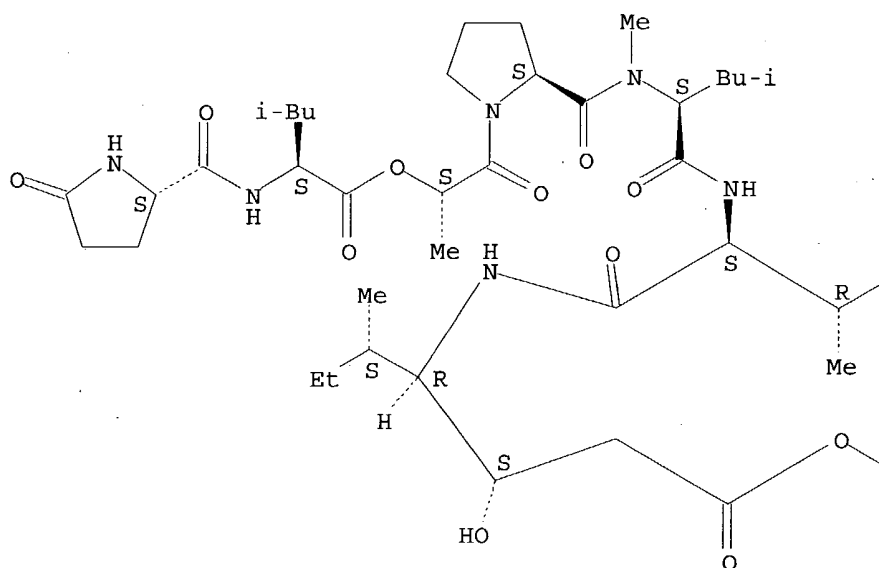


RN 367507-58-2 HCAPLUS

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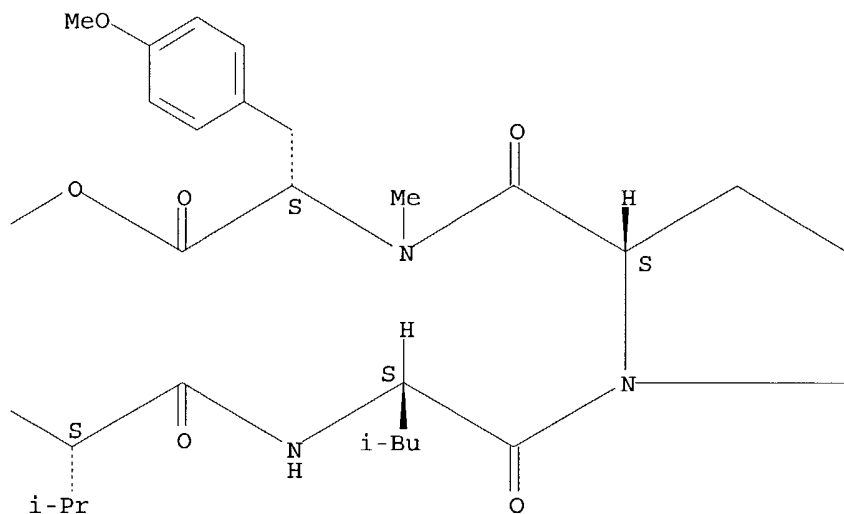
Absolute stereochemistry.

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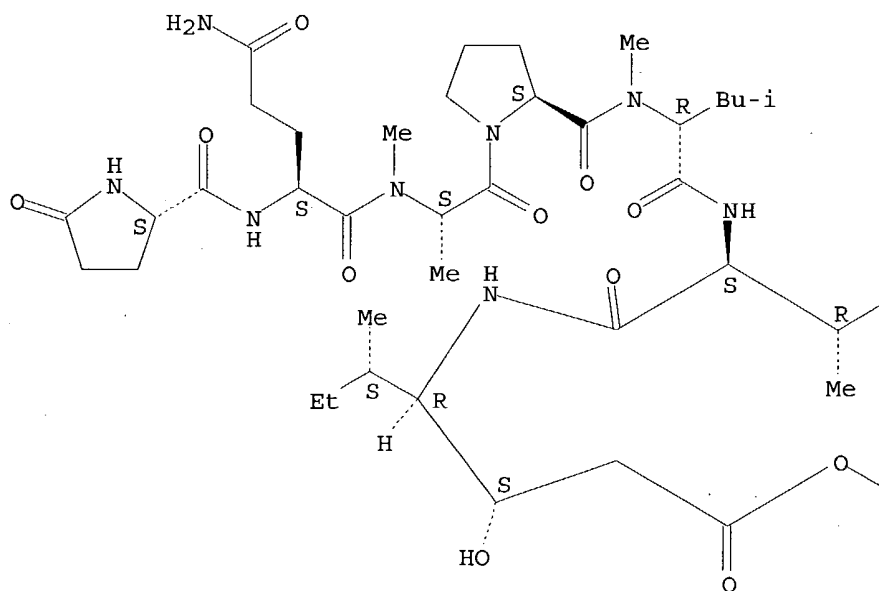


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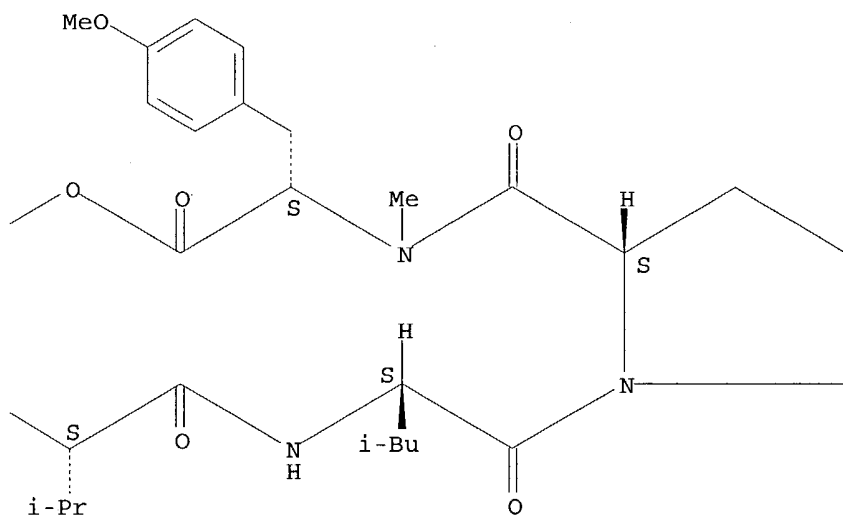
Absolute stereochemistry.

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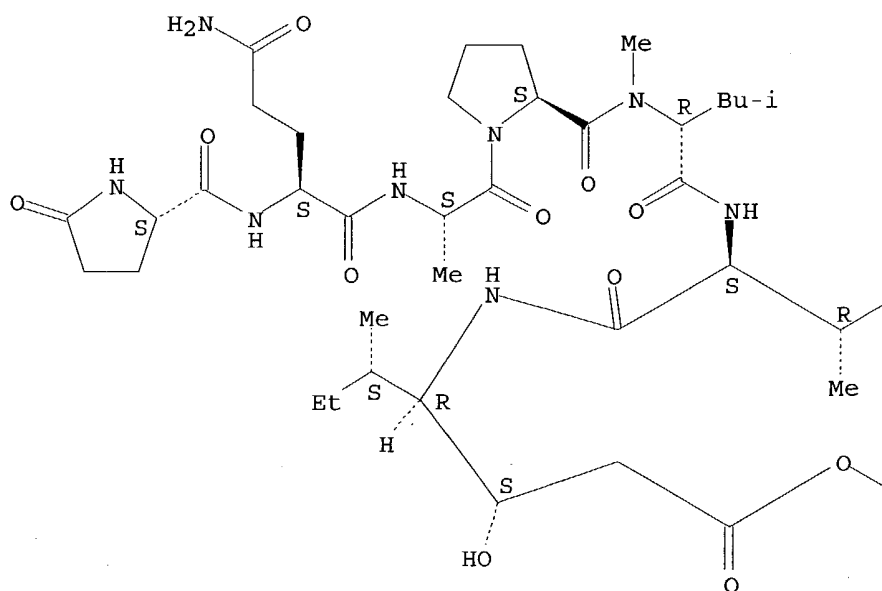


RN 367507-60-6 HCAPLUS

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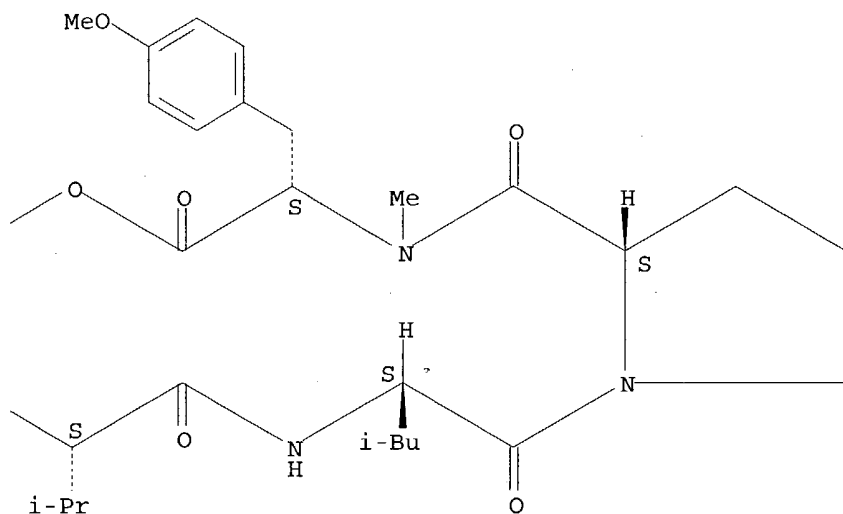
Absolute stereochemistry.

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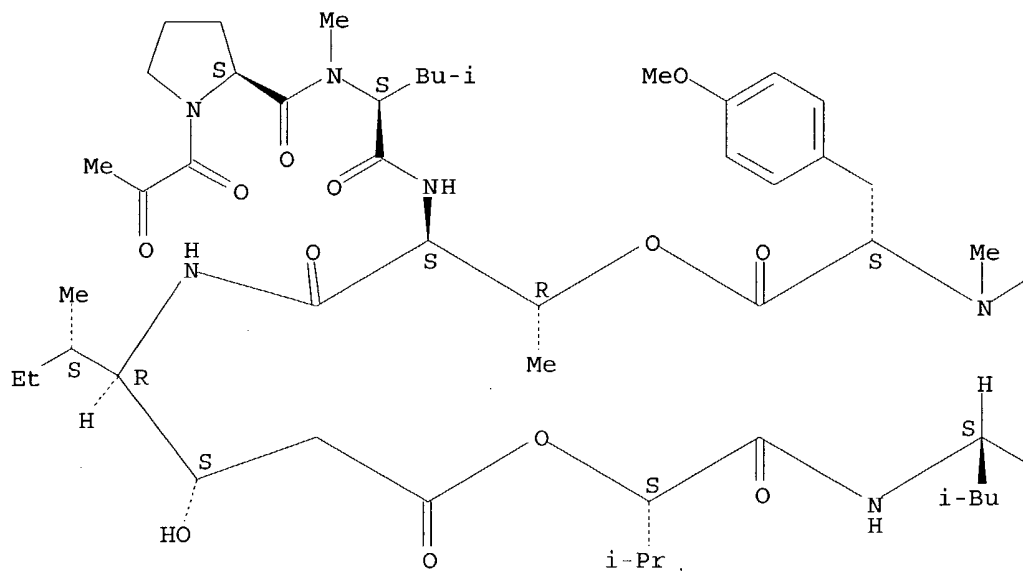


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 (3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-  
 methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (8→3)-lactone (9CI)  
 (CA INDEX NAME)

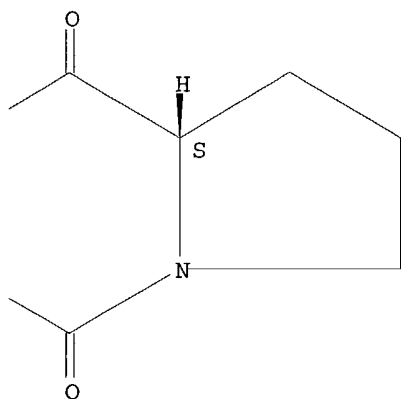
Absolute stereochemistry.

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Searched by P. Ruppel

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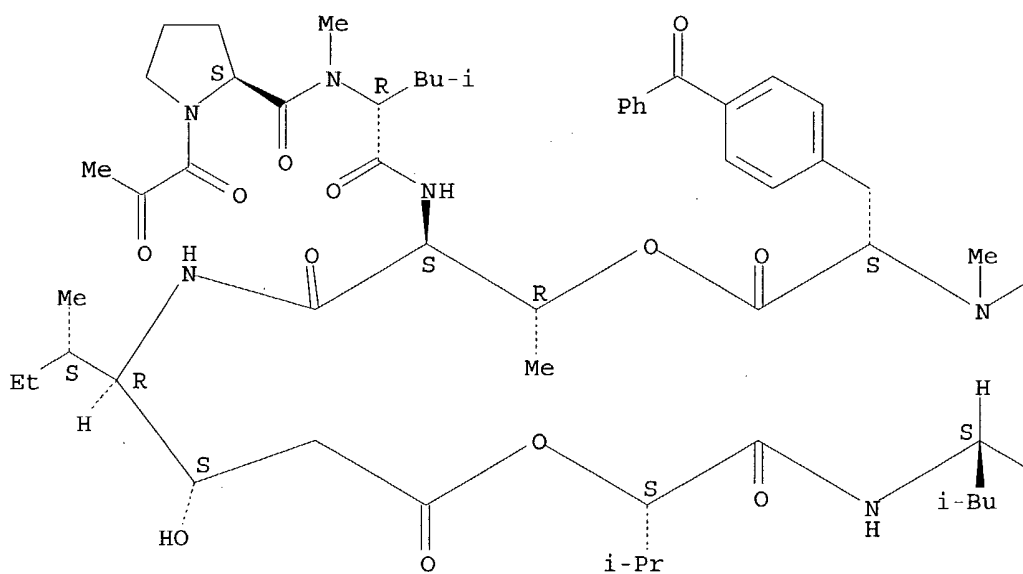


RN 367507-62-8 HCAPLUS

CN L-Phenylalanine, 1-(1,2-dioxopropyl)-L-prolyl-N-methyl-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-4-benzoyl-N-methyl-, (8→3)-lactone (9CI) (CA INDEX NAME)

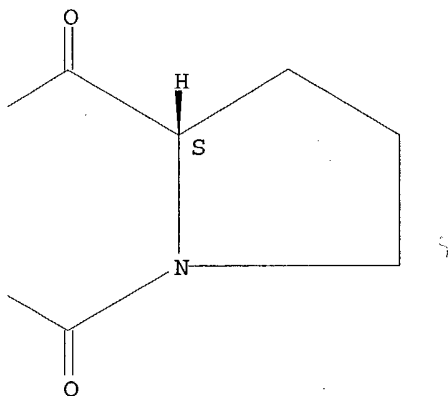
Absolute stereochemistry.

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RN 367507-63-9 HCAPLUS

CN 3-Isoquinolinecarboxylic acid, 1-(1,2-dioxopropyl)-L-prolyl-N-methyl-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxybutanoyl-L-leucyl-L-prolyl-1,2,3,4-tetrahydro-7-methoxy-, (8→3)-lactone, (3S)- (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

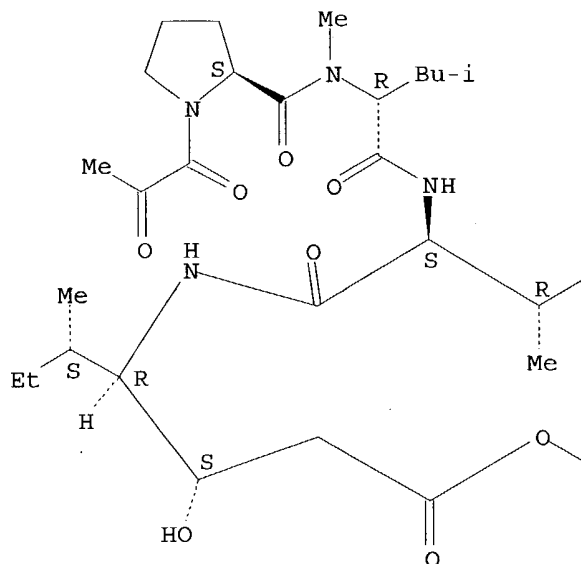
RN 367507-64-0 HCAPLUS

CN L-Tyrosine, 1-(1,2-dioxopropyl)-L-prolyl-N-methyl-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-lysyl-L-prolyl-N,O-dimethyl-, (8→3)-lactone (9CI) (CA INDEX NAME)

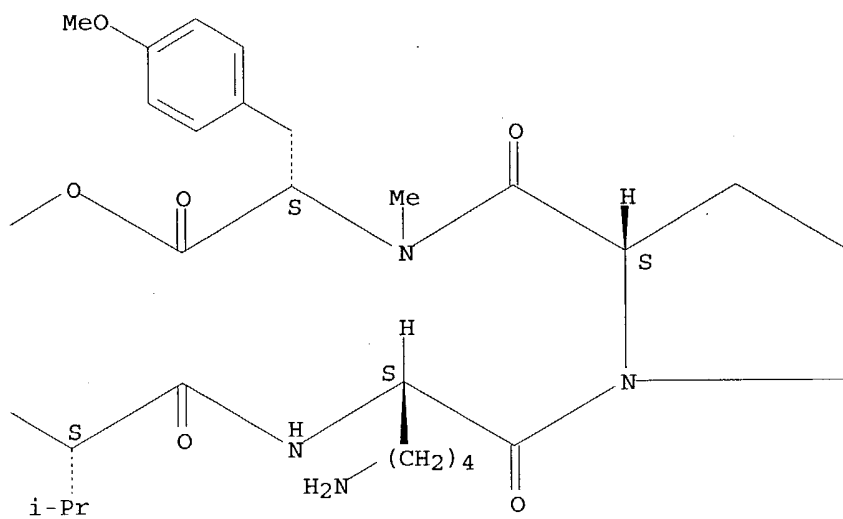
Absolute stereochemistry.



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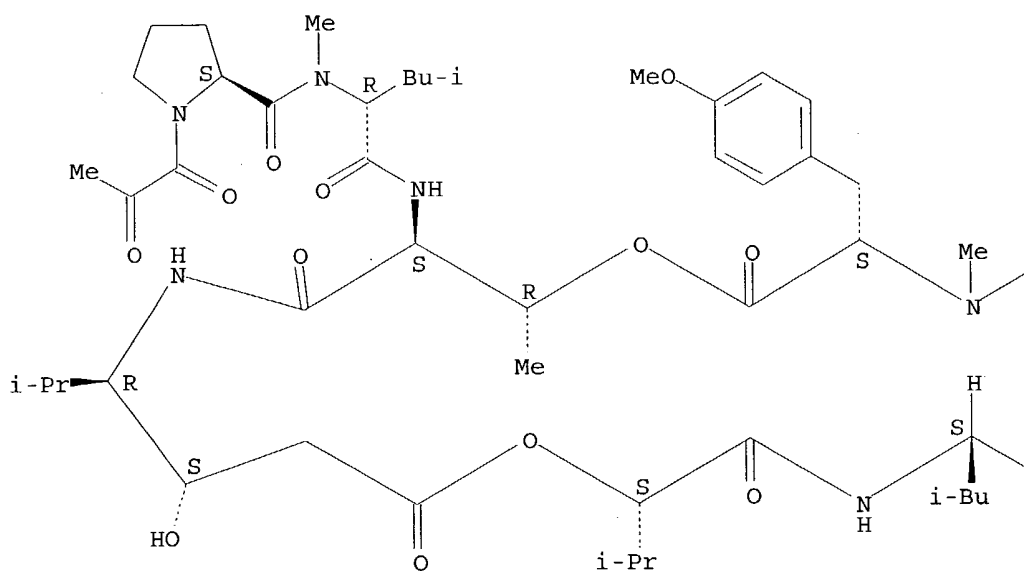
RN 367507-65-1 HCAPLUS

CN L-Tyrosine, 1-(1,2-dioxopropyl)-L-prolyl-N-methyl-D-leucyl-L-threonyl-  
 (3S,4R)-4-amino-3-hydroxy-5-methylhexanoyl-(2S)-2-hydroxy-3-methylbutanoyl-  
 L-leucyl-L-prolyl-N,O-dimethyl-, (8→3)-lactone (9CI) (CA INDEX  
 NAME)

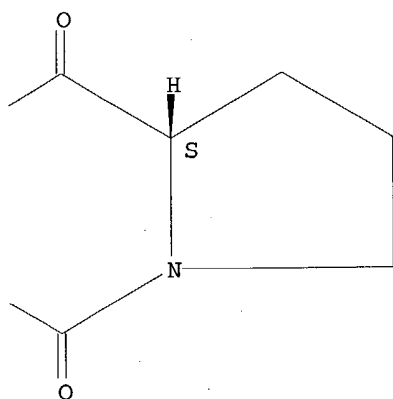
Absolute stereochemistry.

Searched by P. Ruppel

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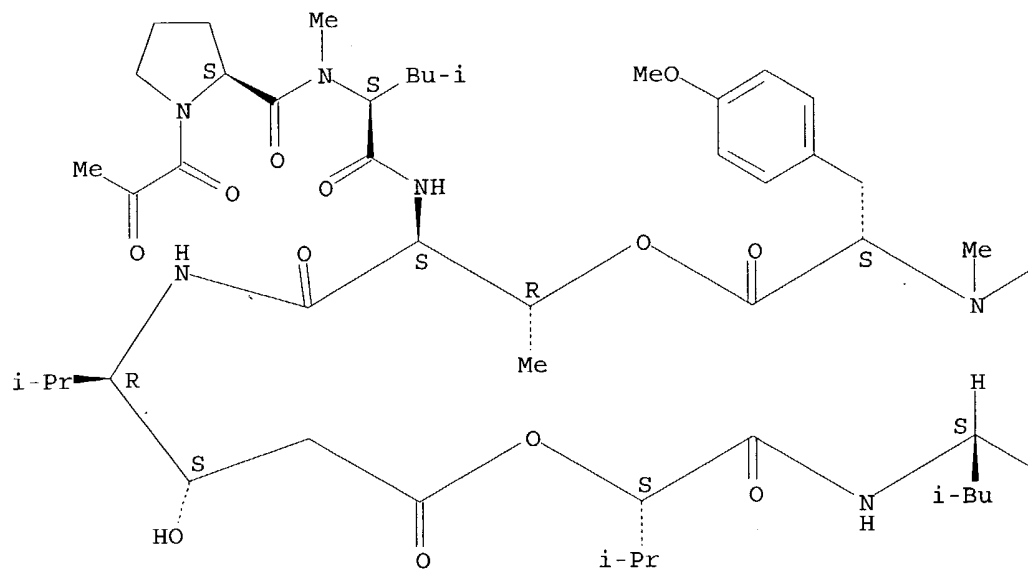
RN 367507-66-2 HCAPLUS

CN L-Tyrosine, 1-(1,2-dioxopropyl)-L-prolyl-N-methyl-L-leucyl-L-threonyl-  
 (3S,4R)-4-amino-3-hydroxy-5-methylhexanoyl-(2S)-2-hydroxy-3-methylbutanoyl-  
 L-leucyl-L-prolyl-N,O-dimethyl-, (8→3)-lactone (9CI) (CA INDEX  
 NAME)

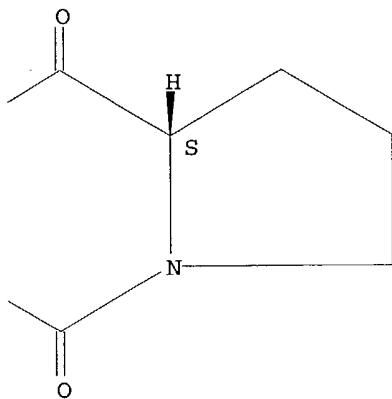
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B



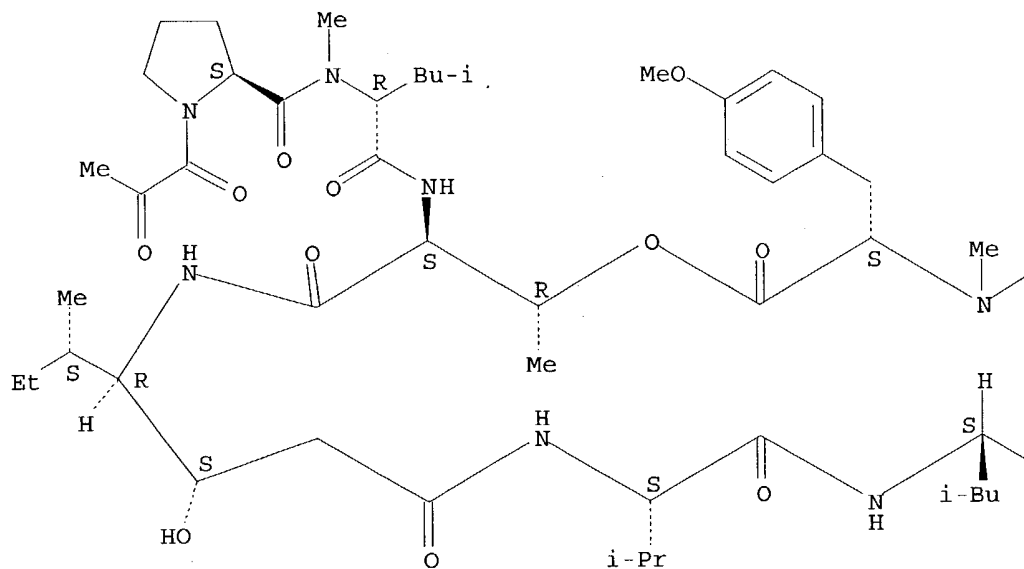
RN 367507-67-3 HCAPLUS

CN 2-9-Tamandarin A, 2-[1-(1,2-dioxopropyl)-L-proline]-6-L-valine- (9CI) (CA INDEX NAME)

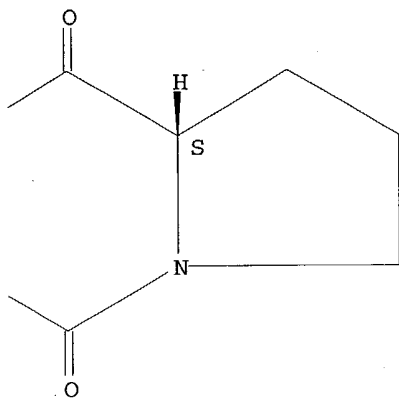
Absolute stereochemistry.

Searched by P. Ruppel

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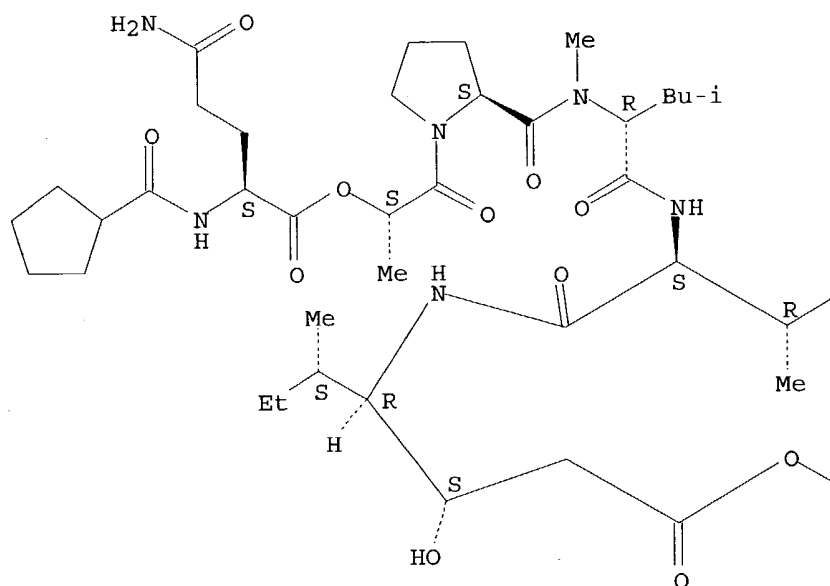
RN 367939-75-1 HCAPLUS

CN L-Tyrosine, N2-(cyclopentylcarbonyl)-L-glutaminyl-(2S)-2-hydroxypropanoyl-L-prolyl-N-methyl-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (10→5)-lactone (9CI) (CA INDEX NAME)

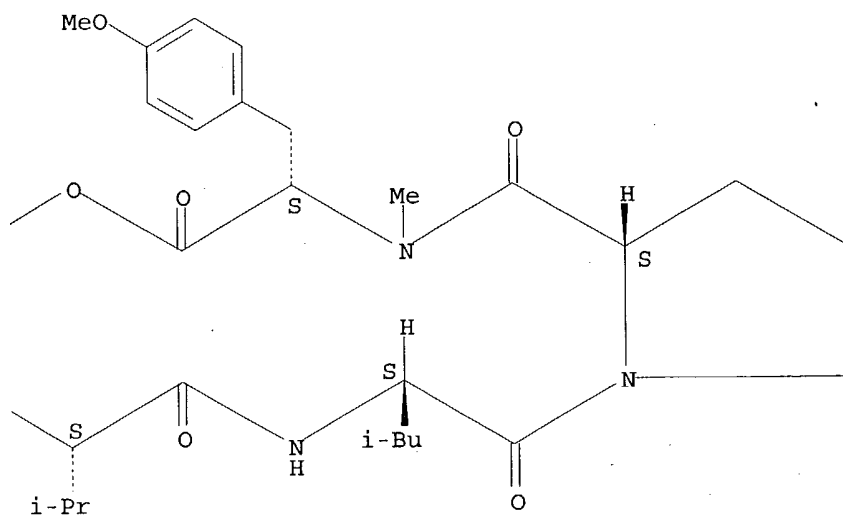
Absolute stereochemistry.

Searched by P. Ruppel

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IT 250039-55-5P 291772-83-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of tamandarin and didemnin analogs)

RN 250039-55-5 HCAPLUS

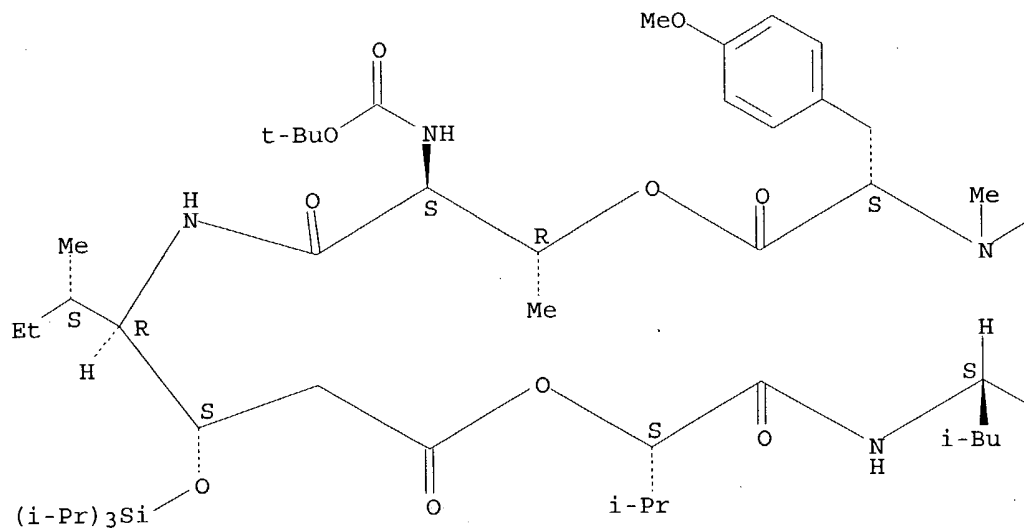
CN 4-9-Tamandarin A, N-[(1,1-dimethylethoxy)carbonyl]-5-[(3S,4R,5S)-4-amino-5-methyl-3-[[tris(1-methylethyl)silyl]oxy]heptanoic acid]- (9CI) (CA INDEX

Searched by P. Ruppel

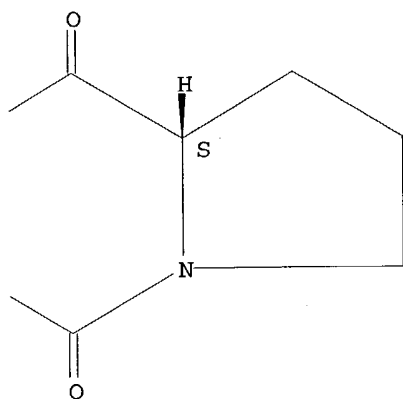
NAME)

Absolute stereochemistry.

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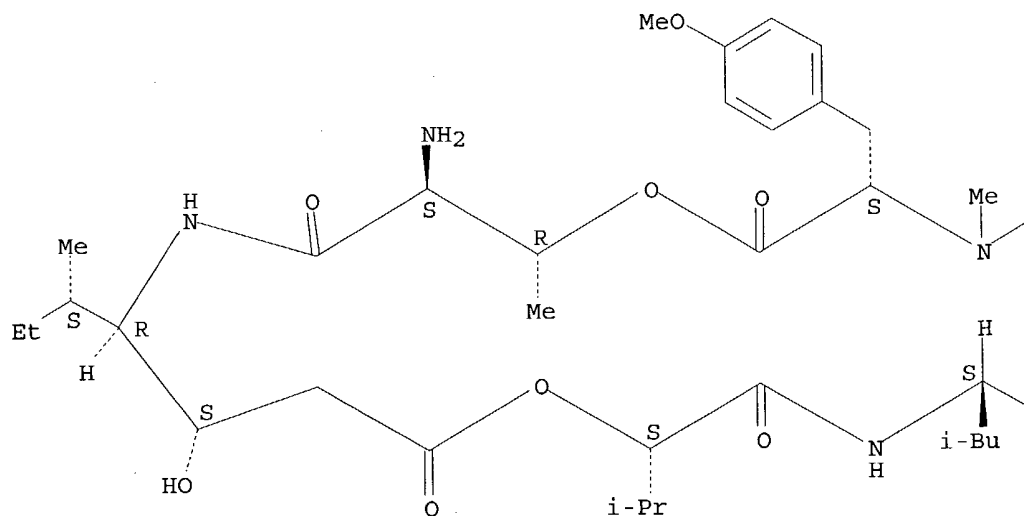
RN 291772-83-3 HCAPLUS

CN L-Tyrosine, L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-  
 2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-,  
 (6-1)-lactone, monohydrochloride (9CI) (CA INDEX NAME)

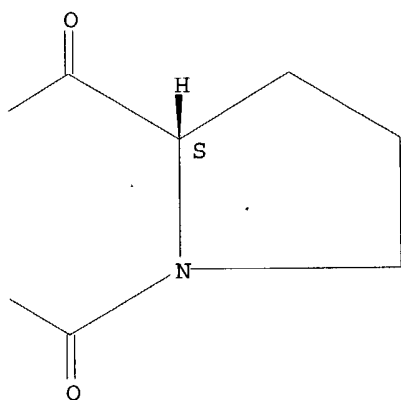
Absolute stereochemistry.

Searched by P. Ruppel

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PAGE 1-B



● HCl

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L62 ANSWER 5 OF 10 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:268658 HCAPLUS

DOCUMENT NUMBER: 135:61525

TITLE: Total syntheses and biological investigations of

tamandarins A and B and tamandarin A analogs

AUTHOR(S): Liang, Bo; Richard, David J.; Portonovo, Padma S.;

Joullie, Madeleine M.

CORPORATE SOURCE: Department of Chemistry, University of Pennsylvania,  
Philadelphia, PA, 19104-6323, USA

Searched by P. Ruppel

SOURCE: Journal of the American Chemical Society (2001),  
123(19), 4469-4474  
CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:61525

AB Tamandarins A (1) and B (2), two natural products similar in structure to didemnin B (3), were recently isolated from a Brazilian marine ascidian of the family Didemnidae. The cytotoxicity of 1 was reported to be somewhat more potent in vitro than that of 3 against various human cancer cell lines. The present account describes the first total syntheses of 1 and 2, and the syntheses of tamandarin A side chain analogs. The cytotoxicity data for these compds. show that the side chain modifications exhibit a parallel effect for both didemnins and tamandarins. This observation supports tamandarins' role as didemnins' mimic.

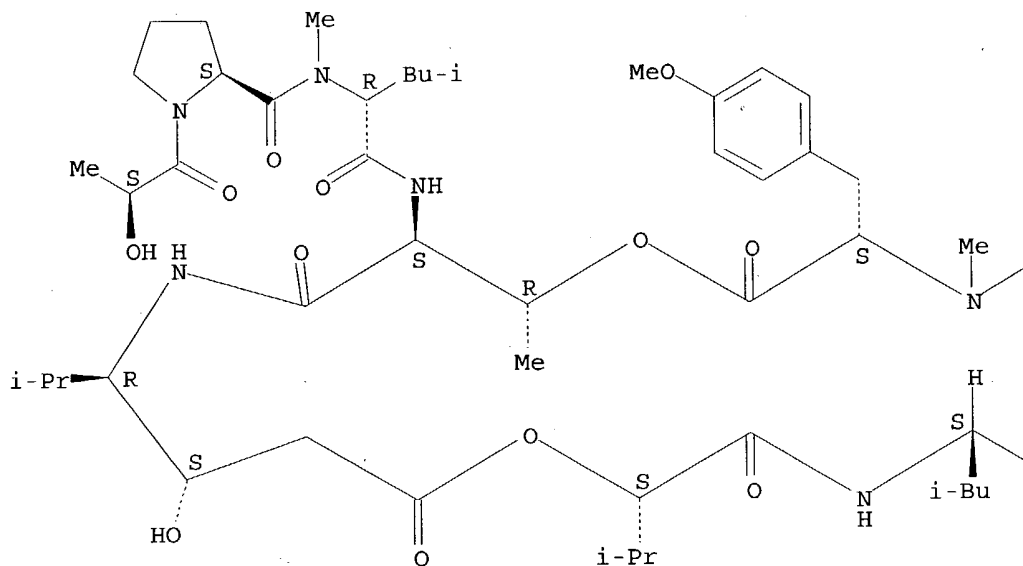
IT 258339-38-7P, Tamandarin B  
RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)  
(preparation and cytotoxicity of tamandarin A, tamandarin B, tamandarin A analogs and didemnin analogs)

RN 258339-38-7 HCAPLUS

CN Tamandarin B (9CI) (CA INDEX NAME)

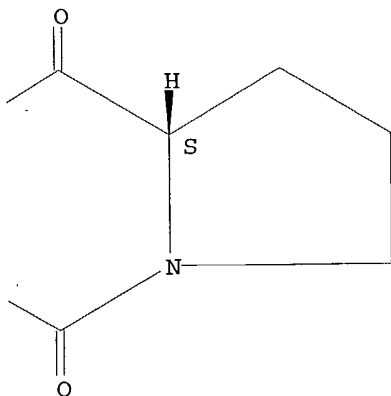
Absolute stereochemistry. Rotation (-).

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IT 291772-81-1

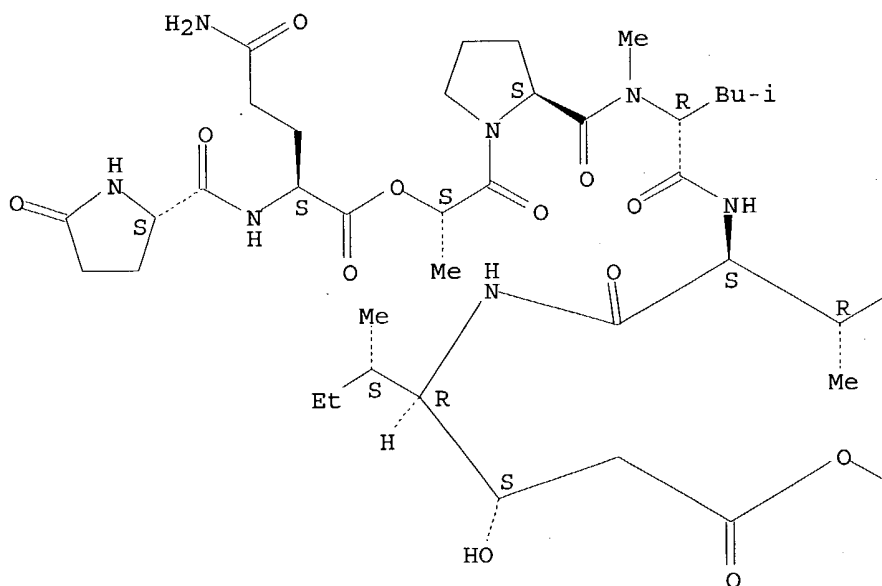
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)  
 (preparation and cytotoxicity of tamandarin A, tamandarin B, tamandarin A analogs and didemnin analogs)

RN 291772-81-1 HCAPLUS

CN Didemnin M, 8-[(2S)-2-hydroxy-3-methylbutanoic acid]- (9CI) (CA INDEX NAME)

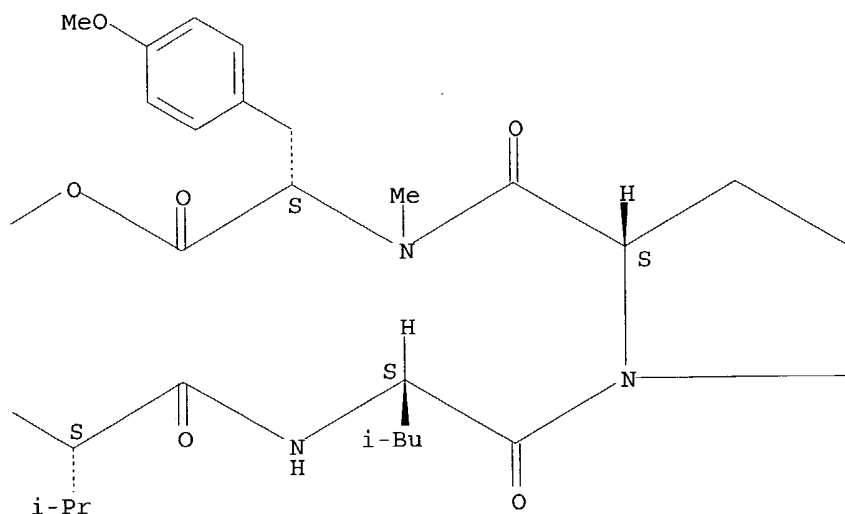
Absolute stereochemistry. Rotation (-).

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Searched by P. Ruppel

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IT 345664-55-3P 345969-81-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

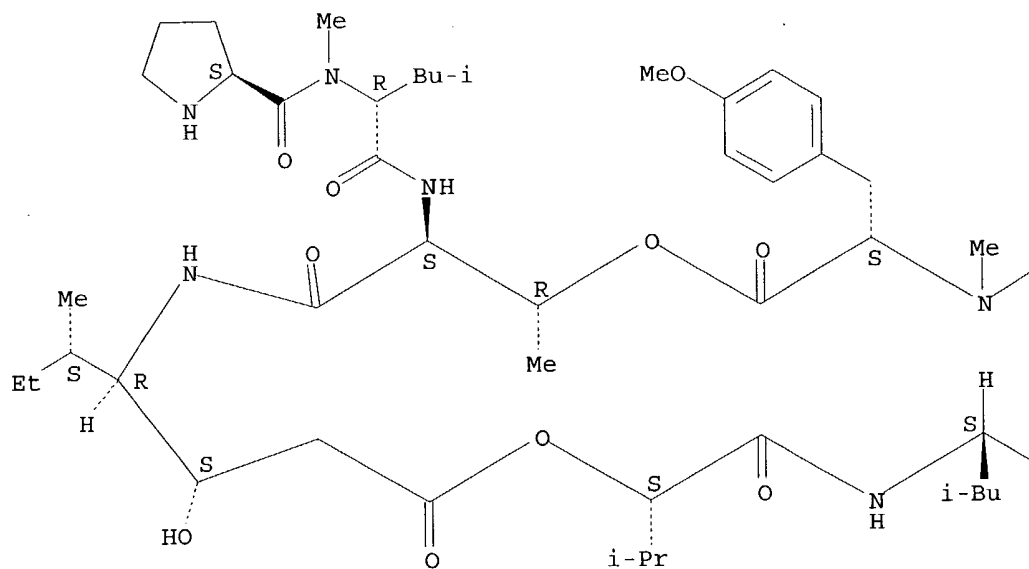
(preparation and cytotoxicity of tamandarin A, tamandarin B, tamandarin A analogs and didemnin analogs)

RN 345664-55-3 HCAPLUS

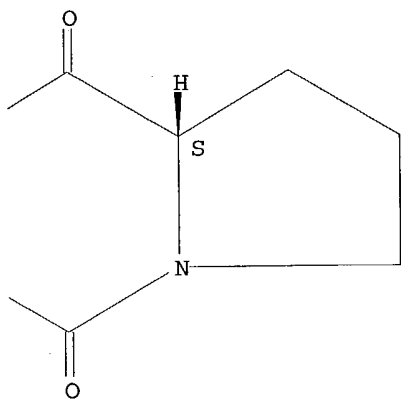
CN L-Tyrosine, L-prolyl-N-methyl-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (8→3)-lactone (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

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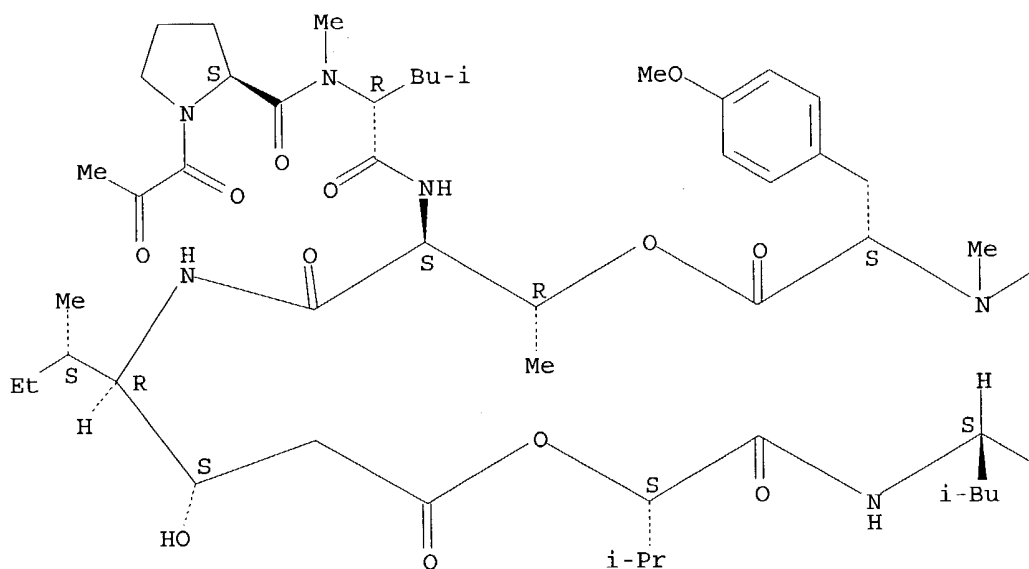


RN 345969-81-5 HCAPLUS  
 CN L-Tyrosine, 1-(1,2-dioxopropyl)-L-prolyl-N-methyl-D-leucyl-L-threonyl-  
 (3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-  
 methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (8→3)-lactone (9CI)  
 (CA INDEX NAME)

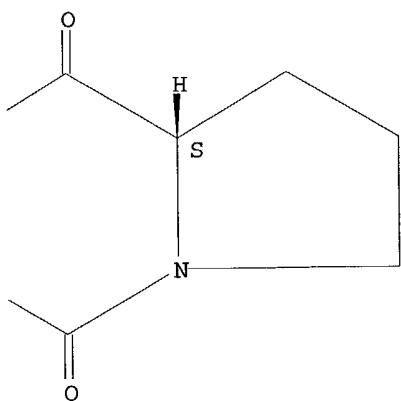
Absolute stereochemistry. Rotation (-).

Searched by P. Ruppel

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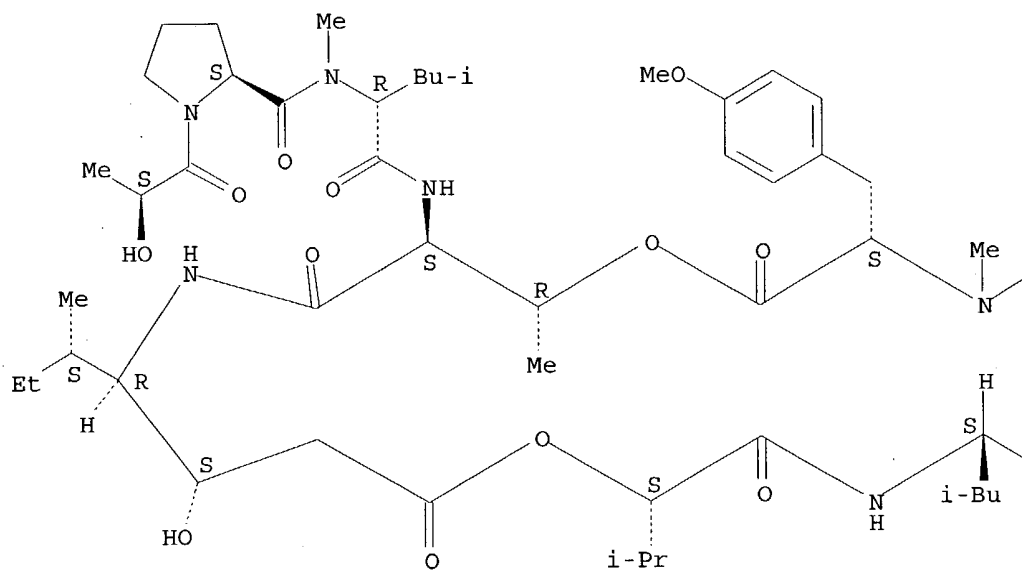


IT 250211-78-0P, Tamandarin A  
 RL: BOC (Biological occurrence); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)  
 (preparation and cytotoxicity of tamandarin A, tamandarin B, tamandarin A analogs and didemnin analogs)  
 RN 250211-78-0 HCAPLUS  
 CN Tamandarin A (9CI) (CA INDEX NAME)

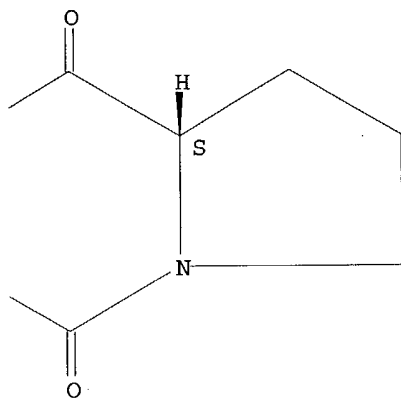
Searched by P. Ruppel

Absolute stereochemistry. Rotation (-).

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IT 250039-55-5P 291772-83-3P 325687-71-6P  
 345664-71-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)

(preparation and cytotoxicity of tamandarin A, tamandarin B, tamandarin A  
 analogs and didemnin analogs)

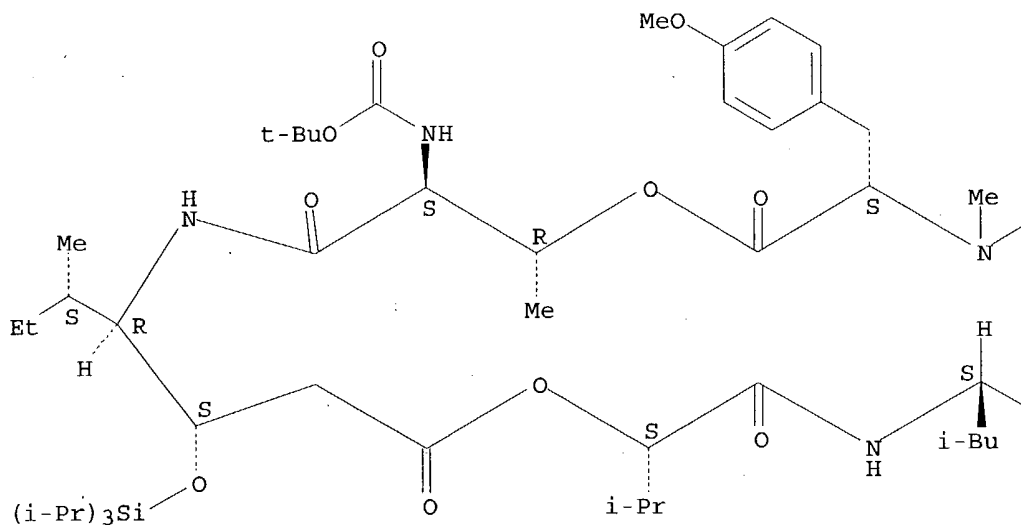
RN 250039-55-5 HCAPLUS

Searched by P. Ruppel

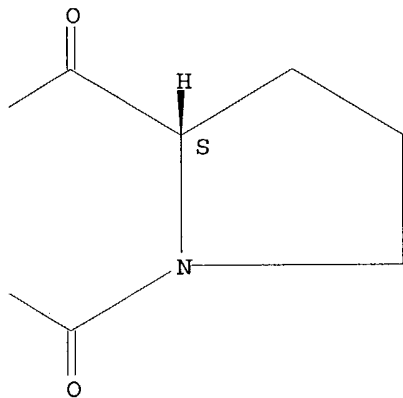
CN 4-9-Tamandarin A, N-[(1,1-dimethylethoxy)carbonyl]-5-[(3S,4R,5S)-4-amino-5-methyl-3-[[tris(1-methylethyl)silyl]oxy]heptanoic acid]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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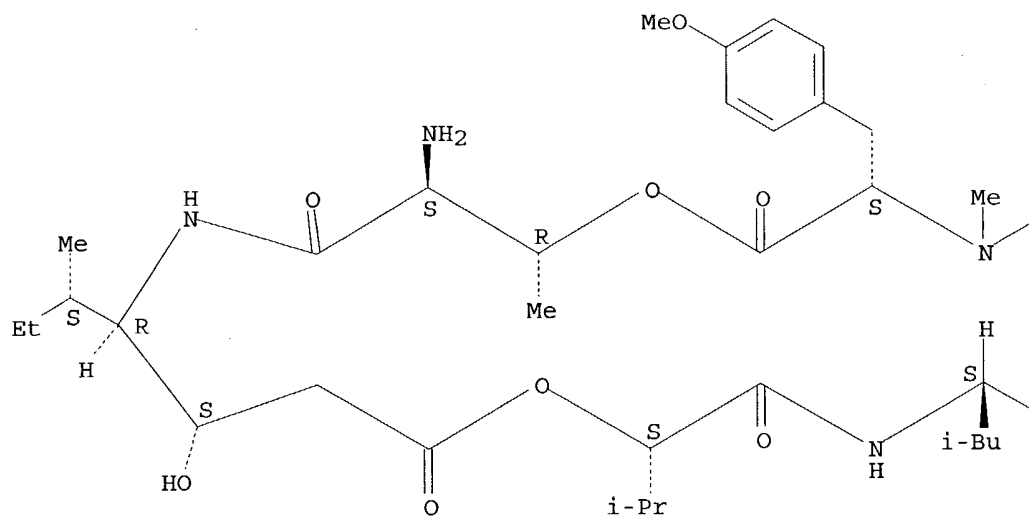
RN 291772-83-3 HCAPLUS

CN L-Tyrosine, L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (6→1)-lactone, monohydrochloride (9CI) (CA INDEX NAME)

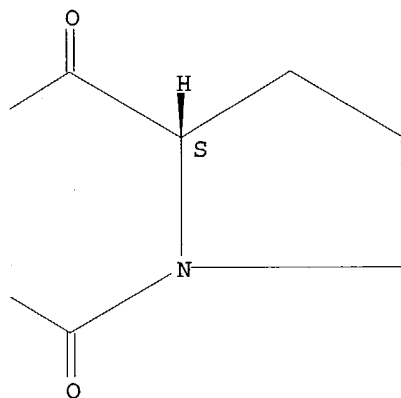
Absolute stereochemistry.

Searched by P. Ruppel

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● HCl

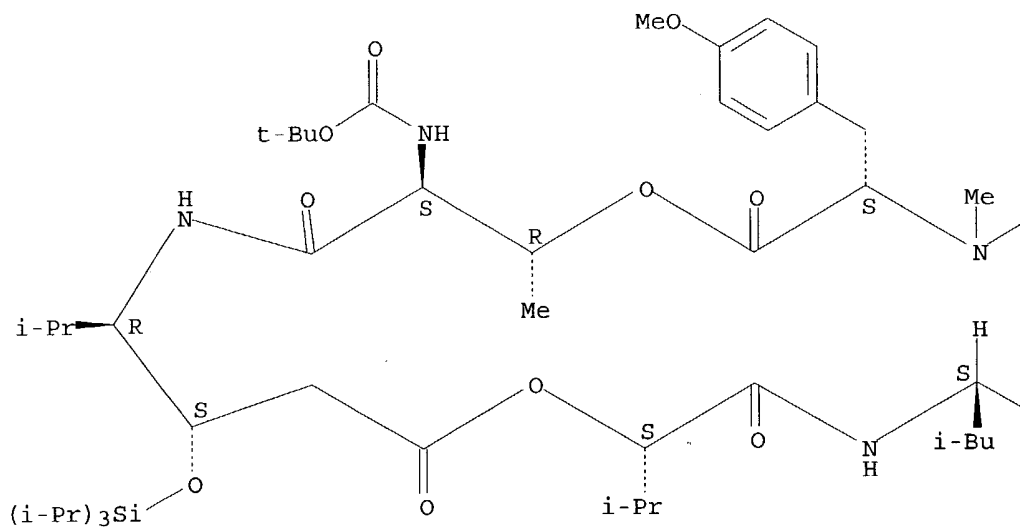
RN 325687-71-6 HCAPLUS

CN L-Tyrosine, N-[(1,1-dimethylethoxy)carbonyl]-L-threonyl-(3S,4R)-4-amino-5-methyl-3-[[[tris(1-methylethyl)silyl]oxy]hexanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (6→1)-lactone (9CI)  
(CA INDEX NAME)

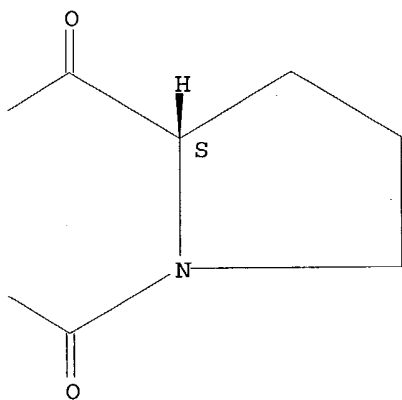
Absolute stereochemistry. Rotation (-).

Searched by P. Ruppel

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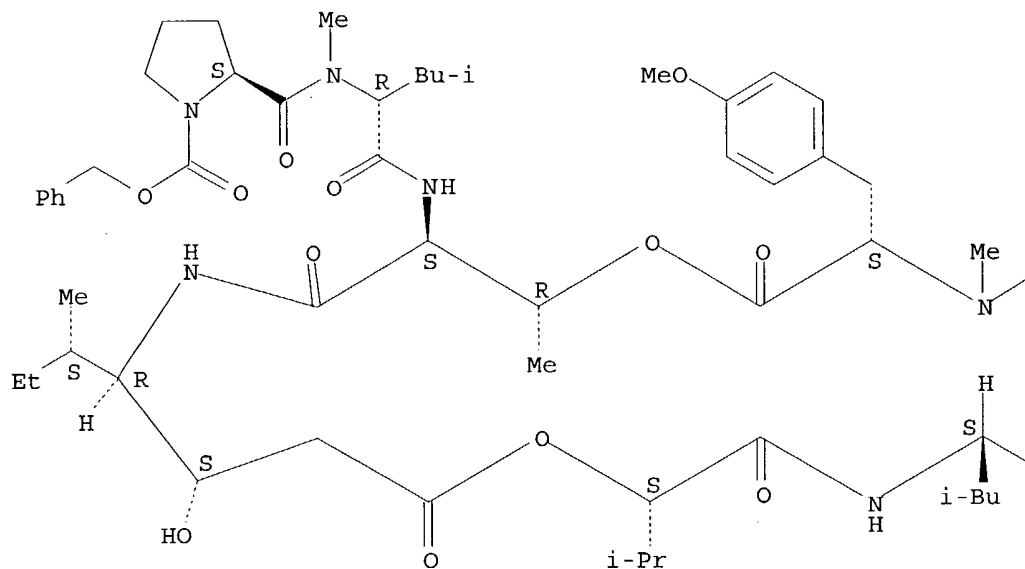


RN 345664-71-3 HCAPLUS  
 CN L-Tyrosine, 1-[(phenylmethoxy)carbonyl]-L-prolyl-N-methyl-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (8→3)-lactone (9CI)  
 (CA INDEX NAME)

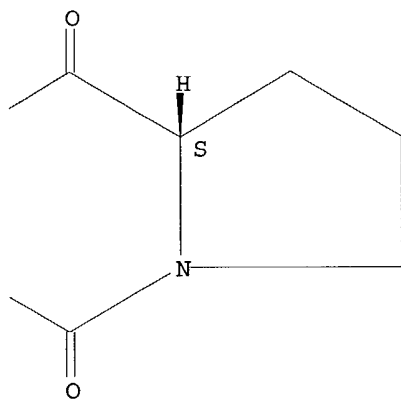
Absolute stereochemistry.



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REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L62 ANSWER 6 OF 10 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2000:897488 HCAPLUS

DOCUMENT NUMBER: 134:163325

TITLE: Total synthesis of (-)-tamandarin B

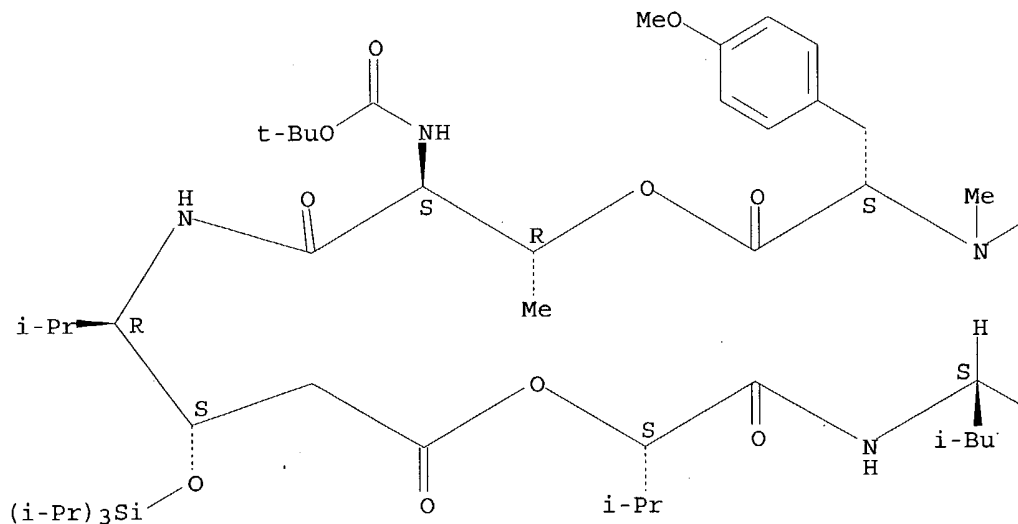
AUTHOR(S): Joullie, M. M.; Portonovo, P.; Liang, B.; Richard, D.

Searched by P. Ruppel

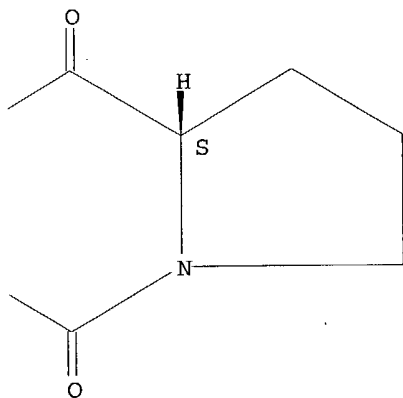
J.  
 CORPORATE SOURCE: Department of Chemistry, University of Pennsylvania,  
 Philadelphia, PA, 19104-6323, USA  
 SOURCE: Tetrahedron Letters (2000), 41(49), 9373-9376  
 CODEN: TELEAY; ISSN: 0040-4039  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 134:163325  
 AB The synthesis of tamandarin B is described. Key steps in the synthesis of  
 the macrocycle component include a diastereoselective ketone reduction, linear  
 precursor formation via an activated pentafluorophenyl ester, and  
 HATU-promoted cyclization. Side-chain coupling was achieved in excellent  
 yield with the newly developed coupling reagent DEPBT.  
 IT **325687-71-6P**  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (total synthesis of cyclic depsipeptide tamandarin B)  
 RN 325687-71-6 HCAPLUS  
 CN L-Tyrosine, N-[(1,1-dimethylethoxy)carbonyl]-L-threonyl-(3S,4R)-4-amino-5-  
 methyl-3-[[tris(1-methylethyl)silyl]oxy]hexanoyl-(2S)-2-hydroxy-3-  
 methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (6→1)-lactone (9CI)  
 (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

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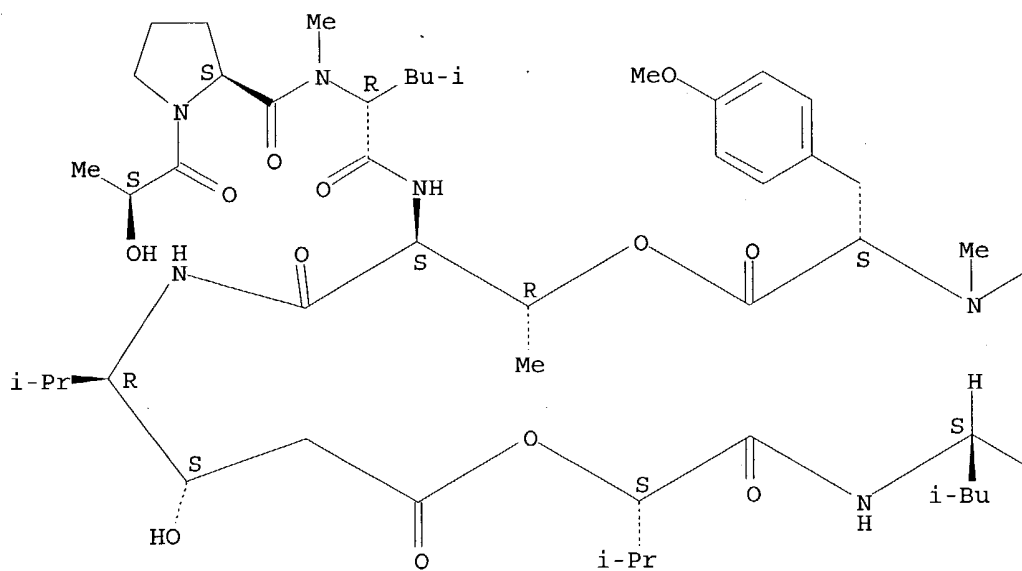
PAGE 1-B



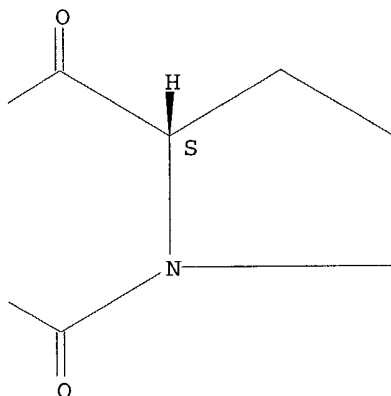
IT 258339-38-7P, Tamandarin B  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (total synthesis of cyclic depsipeptide tamandarin B)  
 RN 258339-38-7 HCAPLUS  
 CN Tamandarin B (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

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REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L62 ANSWER 7 OF 10 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2000:727119 HCAPLUS

DOCUMENT NUMBER: 134:36678

TITLE: Inhibition of protein synthesis by didemnins: cell potency and SAR

AUTHOR(S): Ahuja, Deepika; Geiger, Adam; Ramanjulu, Joshi M.; Vera, Matthew D.; Sir Deshpande, Bhagyashri; Pfizenmayer, Amy; Abazeed, Mohamed; Krosky, Daniel J.; Beidler, David; Joullie, Madeleine M.; Toogood, Peter L.

CORPORATE SOURCE: Willard H. Dow Laboratory Department of Chemistry, University of Michigan, Ann Arbor, MI, 48109-1055, USA

SOURCE: Journal of Medicinal Chemistry (2000), 43(22), 4212-4218

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Synthetic and naturally occurring didemnins are potent and specific inhibitors of protein synthesis in vitro. Structure-activity anal. indicates a requirement for the intact macrocycle; however, the smaller ring size represented by the didemnin analog, tamandarin A, is equipotent to didemnin B. Replacement of the N,O-dimethyltyrosine by a N-methylphenylalanine or N-methylleucine residue is also well-tolerated. The rank order for inhibition of protein synthesis in vitro appears to be retained in MCF-7 cells, albeit at much higher potency. This increase in potency is explained for the first time by data indicating that MCF-7 cells can accumulate didemnin B up to 2-3 orders of magnitude compared to the growth medium.

IT 250211-78-0, Tamandarin A

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

Searched by P. Ruppel

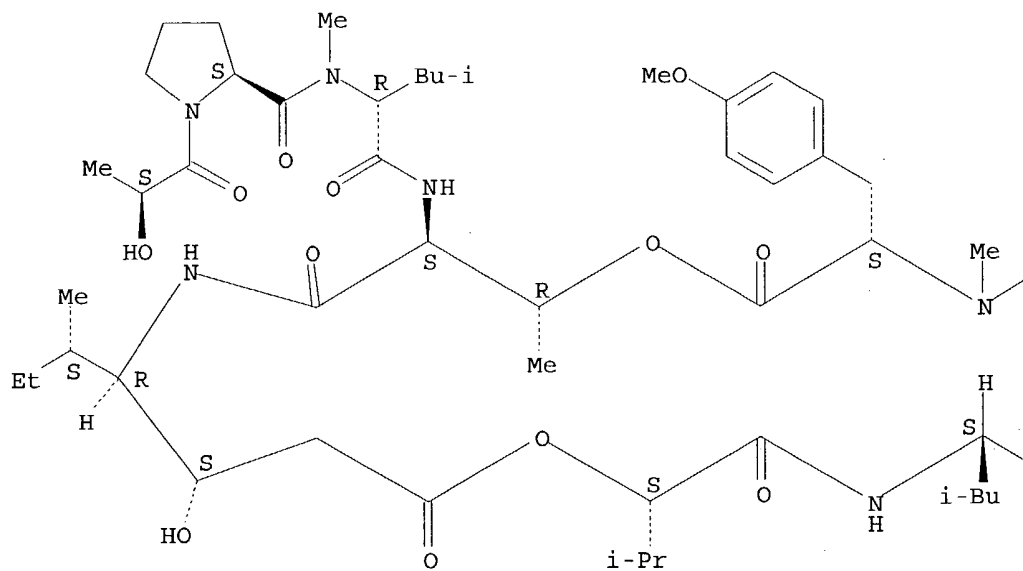
(inhibition of protein synthesis by didemnins and cell potency and SAR)

RN 250211-78-0 HCAPLUS

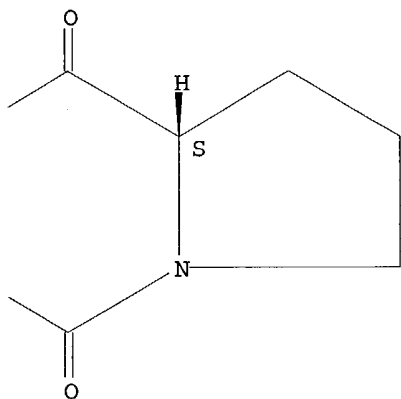
CN Tamandarin A (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

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REFERENCE COUNT:

60

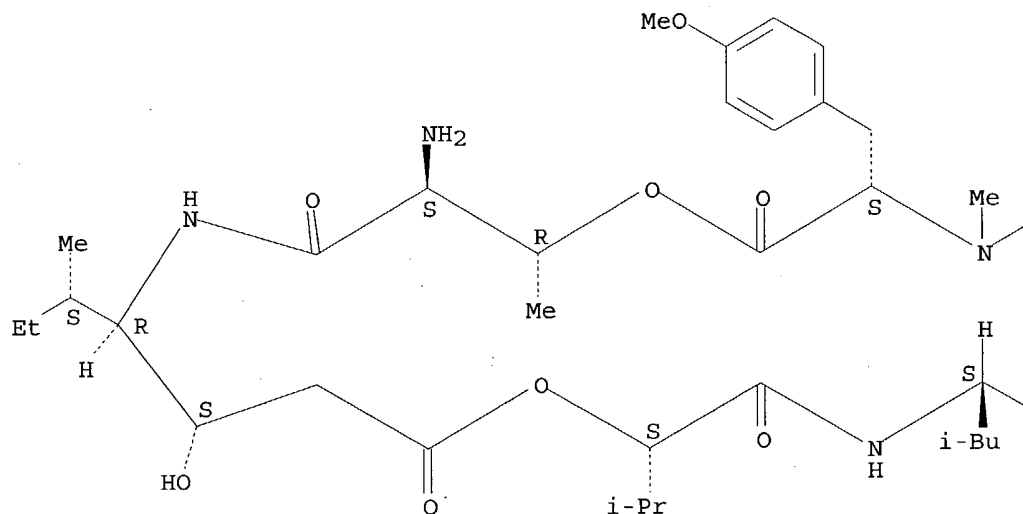
THERE ARE 60 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Searched by P. Ruppel

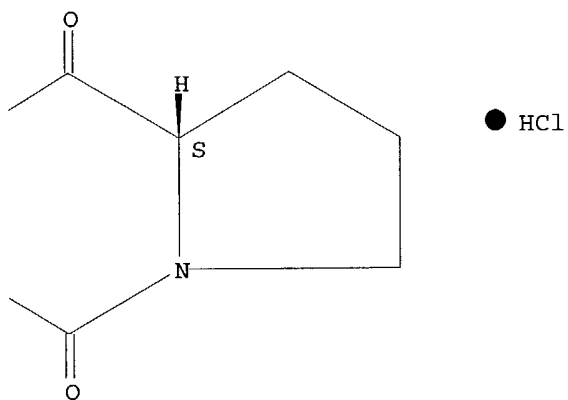
L62 ANSWER 8 OF 10 HCAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 2000:417315 HCAPLUS  
DOCUMENT NUMBER: 133:223009  
TITLE: Total Synthesis of [(2S)-Hiv2]Didemnin M  
AUTHOR(S): Liang, Bo; Vera, Matthew D.; Joullie, Madeleine M.  
CORPORATE SOURCE: Department of Chemistry, University of Pennsylvania,  
Philadelphia, PA, 19104-6323, USA  
SOURCE: Journal of Organic Chemistry (2000), 65(15), 4762-4765  
CODEN: JOCEAH; ISSN: 0022-3263  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 133:223009  
AB The synthesis of of [(2S)-Hiv2]didemnin M (Hiv = hydroxyisovaleryl),  
containing both a simplified tamandarin-type macrocycle and the more complex  
side-chain of didemnin M, is reported.  
IT 291772-83-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(total synthesis of (hydroxyisovaleryl)didemnin M)  
RN 291772-83-3 HCAPLUS  
CN L-Tyrosine, L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-  
2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-,  
(6→1)-lactone, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



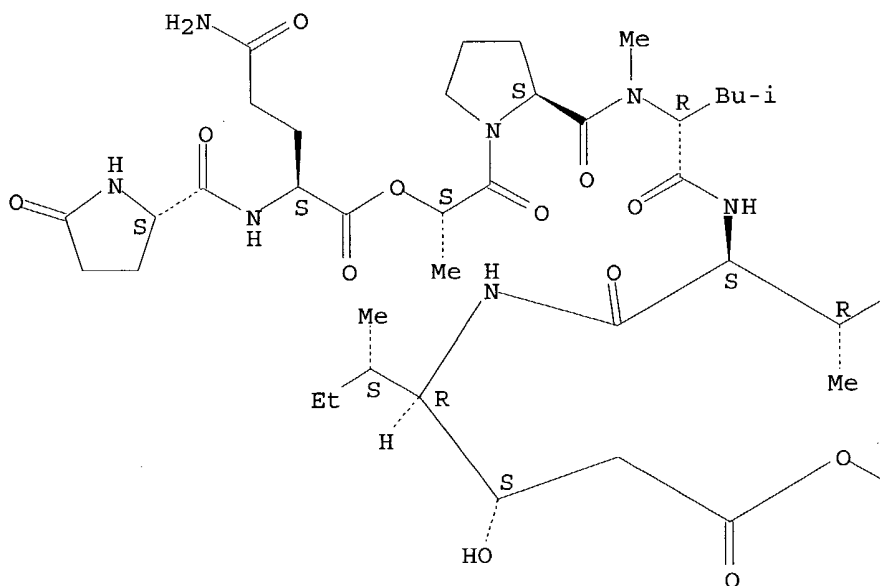
PAGE 1-B



IT 291772-81-1P, [(2S)-Hiv2]Didemnin M  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (total synthesis of (hydroxyisovaleryl)didemnin M)  
 RN 291772-81-1 HCAPLUS  
 CN Didemnin M, 8-[(2S)-2-hydroxy-3-methylbutanoic acid]- (9CI) (CA INDEX  
 NAME)

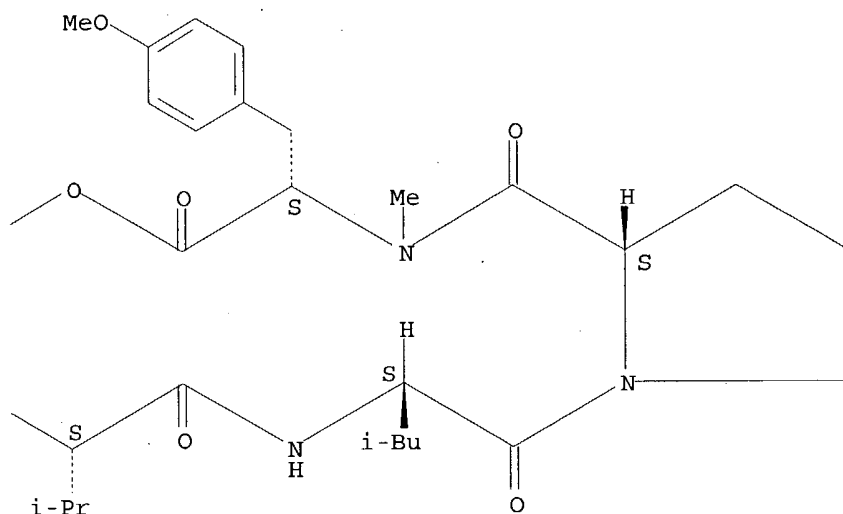
Absolute stereochemistry. Rotation (-).

PAGE 1-A



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PAGE 1-B



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L62 ANSWER 9 OF 10 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:816199 HCAPLUS

DOCUMENT NUMBER: 132:149193

TITLE: Tamandarins A and B: new cytotoxic depsipeptides from a Brazilian ascidian of the family Didemnidae

AUTHOR(S): Vervoort, Helene; Fenical, William; de Epifanio, Rosangela

CORPORATE SOURCE: Center for Marine Biotechnology and Biomedicine  
Scripps Institution of Oceanography, University of  
California-San Diego, La Jolla, CA, 92093-0204, USA

SOURCE: Journal of Organic Chemistry (2000), 65(3), 782-792  
CODEN: JOCEAH; ISSN: 0022-3263

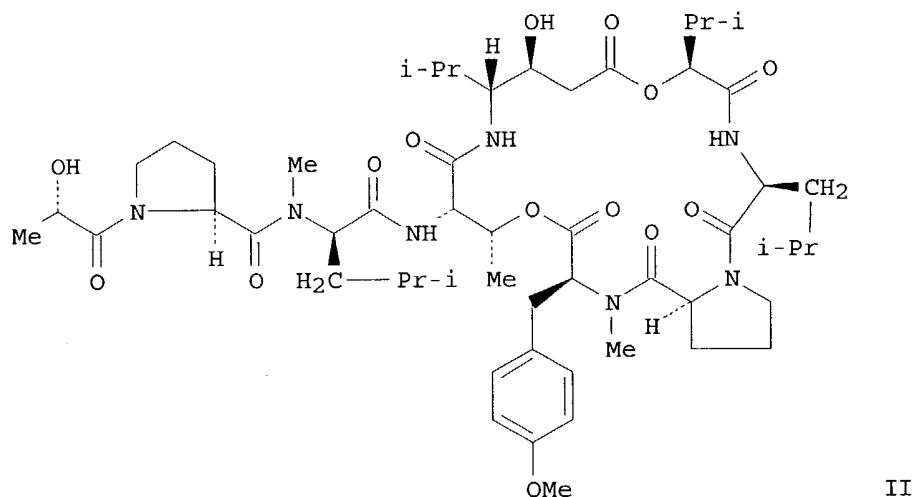
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

GI





AB The structures of two new, naturally occurring cytotoxic depsipeptides, tamandarins A(I) and B (II), are presented. The tamandarins were isolated from an unidentified Brazilian marine ascidian of the family Didemnidae. The structures of the new cytotoxins were assigned by interpretation of FABMS data and by extensive 2D NMR analyses. The absolute configurations of the tamandarins were assigned by acid and alkaline hydrolysis to yield their corresponding amino acids, which were then analyzed as their Marfey derivs. The cytotoxicity of I was evaluated against various human cancer cell lines and shown to be slightly more potent than didemnins B. A qual. discussion of the conformation of I in solution, obtained from NMR J-value data, variable temperature expts., and NOESY/ROESY data, is included.

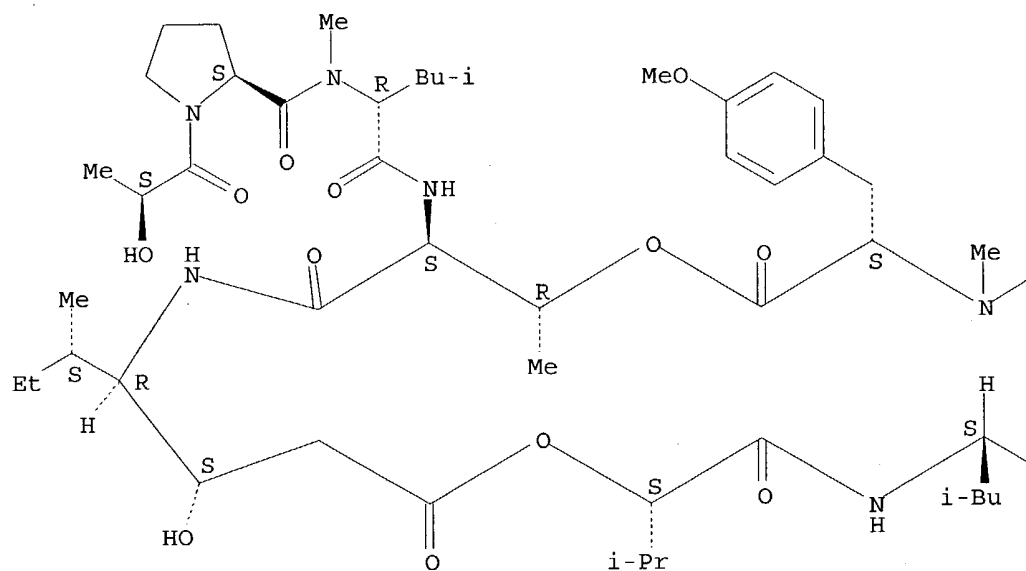
IT 250211-78-0P, Tamandarin A 258339-38-7P, Tamandarin B  
 RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)  
 (cytotoxic depsipeptides from ascidian)

RN 250211-78-0 HCAPLUS

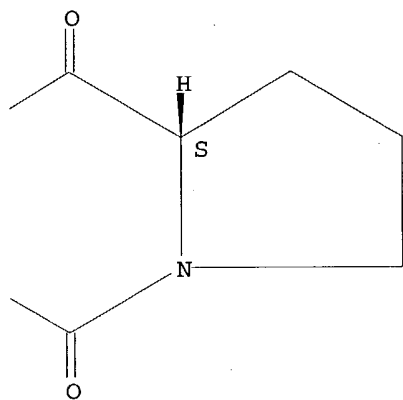
CN Tamandarin A (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

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PAGE 1-B

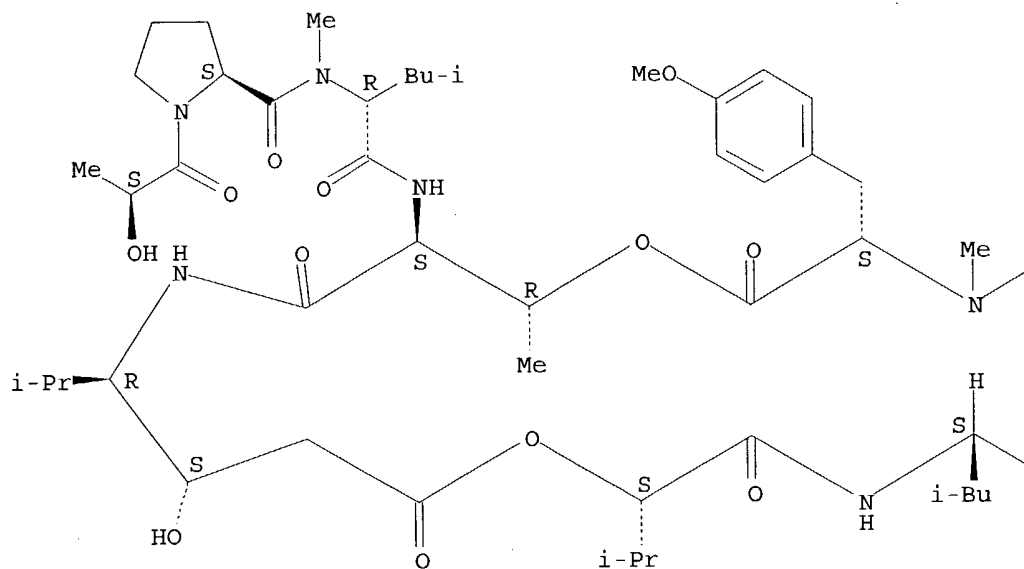


RN 258339-38-7 HCAPLUS  
CN Tamandarin B (9CI) (CA INDEX NAME)

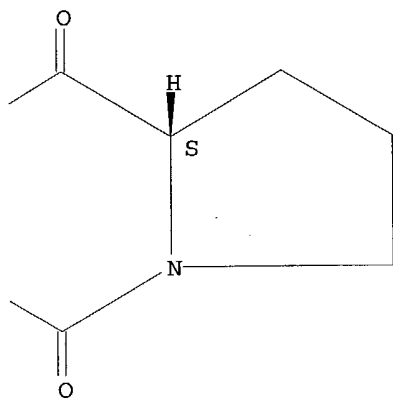
Absolute stereochemistry. Rotation (-).

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 90 THERE ARE 90 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L62 ANSWER 10 OF 10 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:583956 HCAPLUS

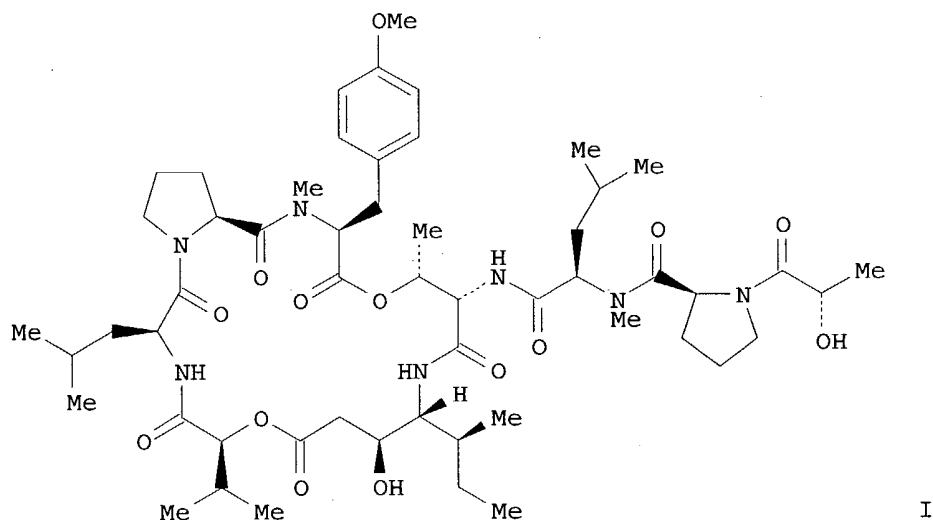
DOCUMENT NUMBER: 131:337334

TITLE: The first total synthesis of (-)-Tamandarin A

AUTHOR(S): Liang, Bo; Portonovo, Padma; Vera, Matthew D.; Xiao,

Searched by P. Ruppel

CORPORATE SOURCE: Dong; Joullie, Madeleine M.  
Department of Chemistry, University of Pennsylvania,  
Philadelphia, PA, 19104-6323, USA  
SOURCE: Organic Letters (1999), 1(8), 1319-1322  
CODEN: ORLEF7; ISSN: 1523-7060  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB Tamandarin A (I), a newly isolated natural product similar in structure to didemnin B, was shown to be somewhat more active in vitro than didemnin B against pancreatic carcinoma with an ED50 value 1.5 to 2 ng/mL. The first total synthesis of I is reported here. The key steps include a practical stereoselective synthesis of the  $\alpha$ -hydroxyisovaleryl-isostatine unit, high-yielding linear precursor formation, a successful macrocyclization, and coupling of the macrocycle with the side chain to afford I.

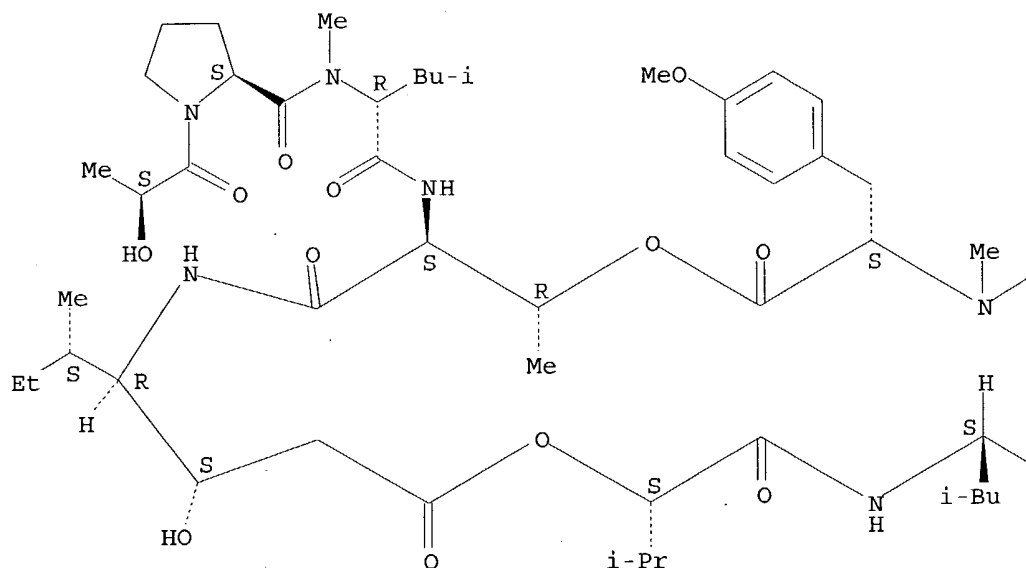
IT 250211-78-0P, Tamandarin A  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
(total synthesis of (-)-Tamandarin A, a naturally occurring anticancer cyclic depsipeptide)

RN 250211-78-0 HCAPLUS

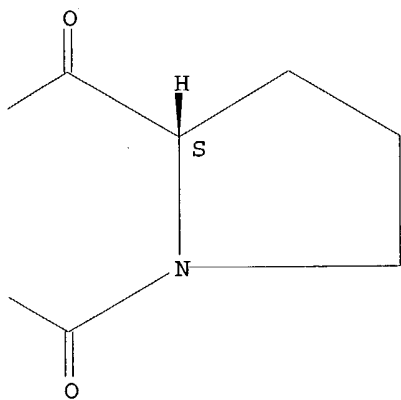
CN Tamandarin A (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

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IT 250039-55-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(total synthesis of (-)-Tamandarin A, a naturally occurring anticancer cyclic depsipeptide)

RN 250039-55-5 HCAPLUS

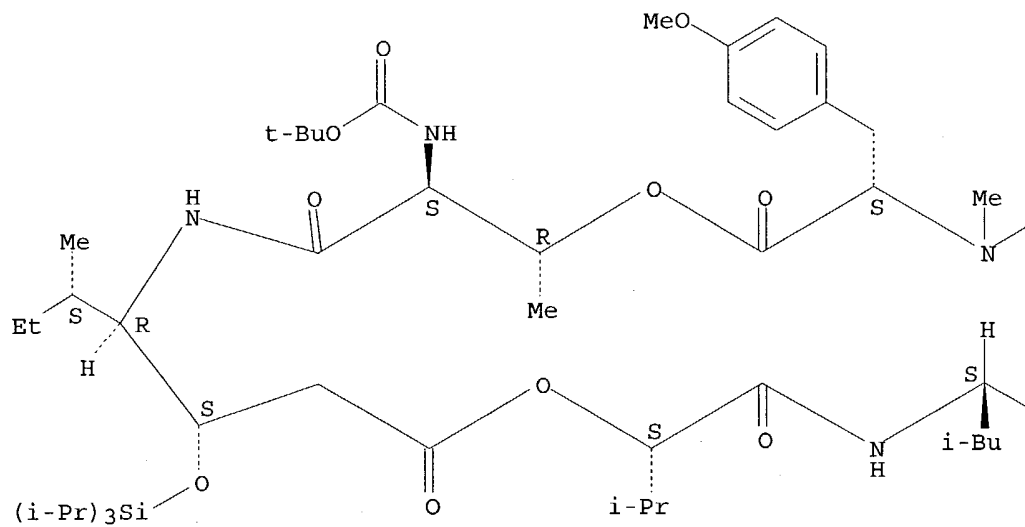
CN 4-9-Tamandarin A, N-[(1,1-dimethylethoxy)carbonyl]-5-[(3S,4R,5S)-4-amino-5-methyl-3-[[tris(1-methylethyl)silyl]oxy]heptanoic acid]- (9CI) (CA INDEX

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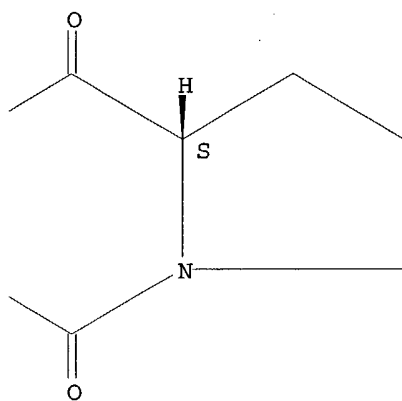
NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



REFERENCE COUNT:

26

THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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FILE 'HOME' ENTERED AT 17:09:37 ON 21 APR 2004

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